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BIOPHYSICAL RESEARCH

AN ANALYSIS OF NUMERICAL MODELS OF AIR POLLUTANT EXPOSURE AND VEGETATION RESPONSE

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EXECUTIVE SUMMARY

A number of empirical (statistical, regression-oriented) and mechanistic (process-oriented) models are presently available to examine the relationship between air pollution stress and plant response.

However, both types of models have their strengths and weaknesses. The experimental and modelling steps in an impact assessment program are closely related; the data collected often dictate the type of model that can be developed or applied, while specifying the use of a given model at the outset will influence the experimentation. In air pollution research, it is common to find these two steps treated separately and even conducted by different researchers, a situation that invariably leads to confusion and conflict between the biological validity of a model and its mathematical representation.

Short-term, acute exposures enable the development of models, represented by a response plane, while long-term, chronic exposures enable the development of models represented by a surface spanning several response planes. Each response plane represents the potential impact of air pollution at a defined plant development stage and response planes will differ in shape because physiologically, for example, a crop will show differential response to a set or similar exposure at different periods of its life. Much of the published literature on air pollutant impacts on agriculture or forestry has not been able to account for this differential response, with scientists simplifying biology by developing a whole season, dose-response statistic. In regression analyses using published data supplied by the original researchers, at least one study has shown that potentially more meaningful impact is assessed using models that recognize the relative importance of growth stages. Many air pollutants occur in a stochastic manner and it is questionable whether whole-season, dose-response functions that are so commonly used have any interpretive value. The policy makers and regulatory personnel prefer a simple approach which would facilitate implementation and administration of ambient air quality standards. Mathematical artifacts introduced through the computation of seasonal dose or through long-term averaging techniques do not make much biological sense. Perhaps an approach which could be meaningful consists of the use of median and percentiles computed from short duration pollutant concentrations and used as input parameters in models which describe chronic effects. Such an approach is free of the influence of the non-normal distribution of the occurrences of pollutant concentrations. However, such a strategy would require the re-computation of much of the data on pollutant exposure kinetics and plant response.

Ecological effects assessed using either of the two groups of models defined in this report will have a degree of uncertainty associated with the quality of data used in the modelling. Empirical-regression models are mainly plot-level models, while explanatory-simulation models are mainly process-level models. In the strictest sense, a model is only applicable at the level from which it is derived, yet we are often faced with making impact assessments at the regional level. This possibility of incurring a scale error is one of the most critical issues facing air pollution researchers interested in impact assessment. There is no general agreement among researchers on how to deal with the scale problem, and while this situation persists, any policy formulated on regional impact assessment must acknowledge the uncertainty.

Recommendations

Based on what is discussed in this report regarding air pollutant exposure and vegetation response, we recommend the following:

1. The way to obtain a simple, single (or few) equation(s) "summary model", possibly for regional scale applications, is to start with a "comprehensive" computer simulation of the biology (all the relevant components and processes, as they are known to function). Presumably, this model would be subjected to field testing, improved if needed and re-tested. Then, it is used to derive the "summary model" equation(s), from the behaviour and sensitivity analysis of variables in the comprehensive model.
2. Summary models should be structured in terms of the probabilities of responses derived from probability density functions of the input parameters and forcing functions.
3. Due to the lack of decisive evidence demonstrating direct vegetation effects induced by acid aerosols or acidic precipitation under field conditions, no models should be considered at this time for these parameters per se. However, they should be included as input parameters in examining other pollutant effects - in other words, examine joint effects.
4. Present pollutant averaging techniques for describing exposure kinetics make neither biological nor mathematical sense. Parameters such as frequency of exposure, peak episodal concentrations, and numerical area under individual exposures should be used as model inputs in defining pollutant exposure kinetics (see Sections 2 and 3).
5. For the purposes of the present study (ADRP), "computer simulation" is required prior to the design of field experiments, data collection, and analysis of air pollutant exposure and vegetation response.
6. For gaseous pollutant effects on plants, the models of Coughenour (1981), SILVA (Kercher and Axelrod 1981), and SUCROS (van Keulen and de Wit 1982) are good starting points. Summaries of these models are described in the Appendices of this report. While these models are mechanistic in nature, they can be adapted into empirical, regression models.

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1. INTRODUCTION

A model can be described as information, data, principles, and the like, arranged or grouped, usually mathematically, so as to represent or describe a certain idea or a condition. In evaluating the impacts of air pollutants on cultivated and native vegetation, a number of investigators have proposed empirical (statistical regression oriented) models (Larsen and Heck 1976; Benson et al. 1982; Heck et al. 1982; Loehman and Wilkinson 1983; Medeiros et al. 1983; Nosal 1983, 1984; and Fox et al. 1986). Others have developed mechanistic (process oriented) models (Ares 1979; Andersson et al. 1980; Haines and Waide 1980; Kercher 1980; Luxmoore 1980; West et al. 1980; Coughenour 1981; Heasley et al. 1981; Kercher and Axelrod 1981; Miller et al. 1982; Harwell and Weinstein 1983; King et al. 1983; and Mortensen 1984). These and other similar models have attempted to explain the relationships between acute or chronic pollutant exposures and vegetation response.

In the present context, "acute exposure" is defined as the occurrence of short-term (few hours to few days), comparatively high pollutant concentrations. On the other hand "chronic exposure" is defined as the occurrence of long-term (weeks, months, entire life cycle of vegetation), comparatively low pollutant concentrations, with periodic, intermittent episodes or peaks. However, there are exceptions to this definition of "chronic exposure". For example, in parts of the United Kingdom the geometric standard deviation of sulphur dioxide concentrations in rural areas is fairly constant (roughly 2.0). This allows the prediction of the duration of exposure to concentrations within defined thresholds, from the air quality monitoring data (Fowler and Cape 1982).

Generally "acute exposures" cause symptoms of injury on vegetation. On the other hand "chronic exposures" may or may not result in symptom production. Depending on the timing of the stress, whole plants can frequently recover from the effects induced by an acute exposure in one part of the plant (e.g., group of leaves which are at a sensitive growth stage), through overall compensatory processes of the entire plant. On the other hand, of greater concern are the effects which result from long-term chronic exposures. Such chronic effects consist of changes in growth, productivity, reproduction, and quality. These effects may or may not be preceded by symptoms of injury. In addition, chronic exposures can result in changes in features relevant to aesthetic and recreational aspects.

The ability to understand and predict temporal and spatial patterns of air pollutant effects on vegetation continues to constitute an important need in agricultural and natural resource management. Thus, in this report we describe and evaluate the state of published mathematical models of air quality and vegetation response. We also identify the limitations in these models and describe some basic biological and statistical concepts of plant response processes useful in experimental design toward a new and progressive approach to the problem analysis.

2. CHARACTERISTICS OF AMBIENT AIR QUALITY

The pollutants in the atmosphere exist as gases, vapours or particles (solid and liquid). The mechanisms for the transfer of these to plant surfaces consist of "dry deposition" (diffusion, brownian motion, impaction and sedimentation) and "wet deposition" (such as rain, snow, and fog). Any resultant vegetation effects observed can be due to direct stress on the plant species, to indirect stress mediated by the soil, or to a combination of both. Torn et al. (1987) and Mayo (1987) have reviewed the published literature on the effects of acidic and acidifying pollutants on crop and tree species, respectively. In evaluating the effects of pollutants under ambient conditions, one must define the spatial and temporal variability. In addition, because of the nature of atmospheric processes, two or more pollutants can exhibit in a 24 hour period, increases or decreases in their concentrations simultaneously, sequentially, inversely, or in some variable or poorly defined pattern relative to each other. For example, in a typical situation of photochemistry, high concentrations of ozone (O_3) and nitric oxide (NO) occur simultaneously, while high concentrations of nitrogen dioxide (NO_2) precede O_3 (NAS 1977). While high concentrations of O_3 are generally observed during daylight hours (the exception being stratospheric intrusion of O_3), high concentrations of fine particle sulphate (SO_4) are observed during nighttime hours (Stevens et al. 1978). Thus, under field conditions, vegetation is first exposed to high concentrations of fine particle SO_4 during the early part of the day and subsequently to high concentrations of O_3 during the late afternoon hours. The significance of this has been demonstrated by Herzfeld (1982) and reviewed by Chevone et al. (1986). When plants were exposed to fine particle SO_4 followed by O_3 under controlled conditions, the injurious effects of O_3 were significantly increased, in comparison to the effects induced by O_3 alone. The aerosol by itself did not produce detectable negative effects. Thus, certain pollutants such as O_3 and sulphur dioxide (SO_2) are known to be relatively more phytotoxic than others and under appropriate conditions exist at sufficient ambient concentrations. Other pollutants such as NO_2 and SO_4 are known to be relatively less phototoxic and do not appear to exist at ambient concentrations sufficient to cause injury. However, what is critical is the joint effect of the two types of pollutants. In addressing this issue not only must one define the comparative relationships of the occurrence patterns of pollutants of concern, but also provide correctly and satisfactorily an appropriate numerical description of frequency distributions and time series analysis of individual pollutant occurrences.

Many scientists assume that the frequency distribution of pollutant concentrations follows a normal, "bell-shaped" distribution. The following is an example of normal distribution: X is said to have the normal distribution if the distribution function of X is given by

$$F(x) = P(X \leq x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}\,\sigma} e^{-1/2[(y-\mu)/\sigma]^2} dy$$

where it can be shown that the parameters μ and σ are the mean and standard deviation of X. The standard normal distribution is the normal distribution with μ equal to 0 and

σ equal to 1 (Snedecor and Cochran 1978). Long-term pollutant averaging techniques assume this (e.g., Oshima et al. 1976; Heagle et al. 1986). In reality, if frequency distributions of the occurrence of O_3 or oxides of nitrogen are plotted graphically (Figure 1), their distribution is skewed with a long tail at high values. This is also true for SO_2 (Table 1). According to Fowler and Cape (1982), if the frequency classes are plotted in terms of the logarithm of SO_2 concentrations, however, then a more symmetrical distribution is obtained, with data from UK. An example of lognormal distribution is:

$$p_x(x) = [(x-\theta)\sqrt{2\pi}\,\sigma]^{-1}\, e^{-1/2[\log(x-\theta)-\zeta]^2)\sigma^2} \quad (x>\theta)$$

A similar conclusion was also reached by Male (1982) in the US.

The assumption of log-normality has been questioned by Berger et al. (1982) in Belgium. These authors used 24-hour averages of SO_2 concentrations over a two and one-half year period in the region of Ghent, Belgium. Lognormal distribution was fitted to the data with poor results. The differences between the empirical data and the log-normal curve were most pronounced at extreme values of the 95th and higher percentiles. For this reason, the authors used the two-parameter gamma distribution:

$$F(x) = \frac{1}{\beta^{\alpha}\Gamma(\alpha)} \int_0^x x^{\alpha-1} \exp\{\frac{X}{\beta}\}dx$$

The gamma distribution provided a much better fit and the goodness-of-fit was confirmed by several tests of significance.

Most recently, Buttazzoni et al. (1986), evaluating the sulphur dioxide concentrations in the area of Venice, Italy concluded that:

1. Their results seem to suggest that 2, 3, or 4-parameter lognormal distributions do not hold characteristics of generality or universality for the interpretation of air quality data;
2. In fact, Weibull and gamma distributions yield superior simulations in Venice;
3. Bell-shaped distributions cannot fit L-shaped experimental data sets; and
4. Gamma distributions are less convenient than Weibull distributions.

According to the authors, as a final comment, "the research for a universal form allowing for direct comparisons among distributions underlined by differing sites or time spans, should head toward a generalization of such distributions".

In addition to the aforementioned studies, Lefohn and Benedict (1982) and Nosal (1984) examined the frequency distribution patterns of ambient O_3 concentration in parts of the US. They concluded that such distributions follow a Weibull function (Figures 1 and 2). An example of Weibull distribution:

$$p_x(x) = c_{\alpha}^{-1}\{(x-\xi_0)/\alpha\}^{c-1} e^{-[(x-\xi_0)/\alpha]^c} \quad (\xi_0<x)$$

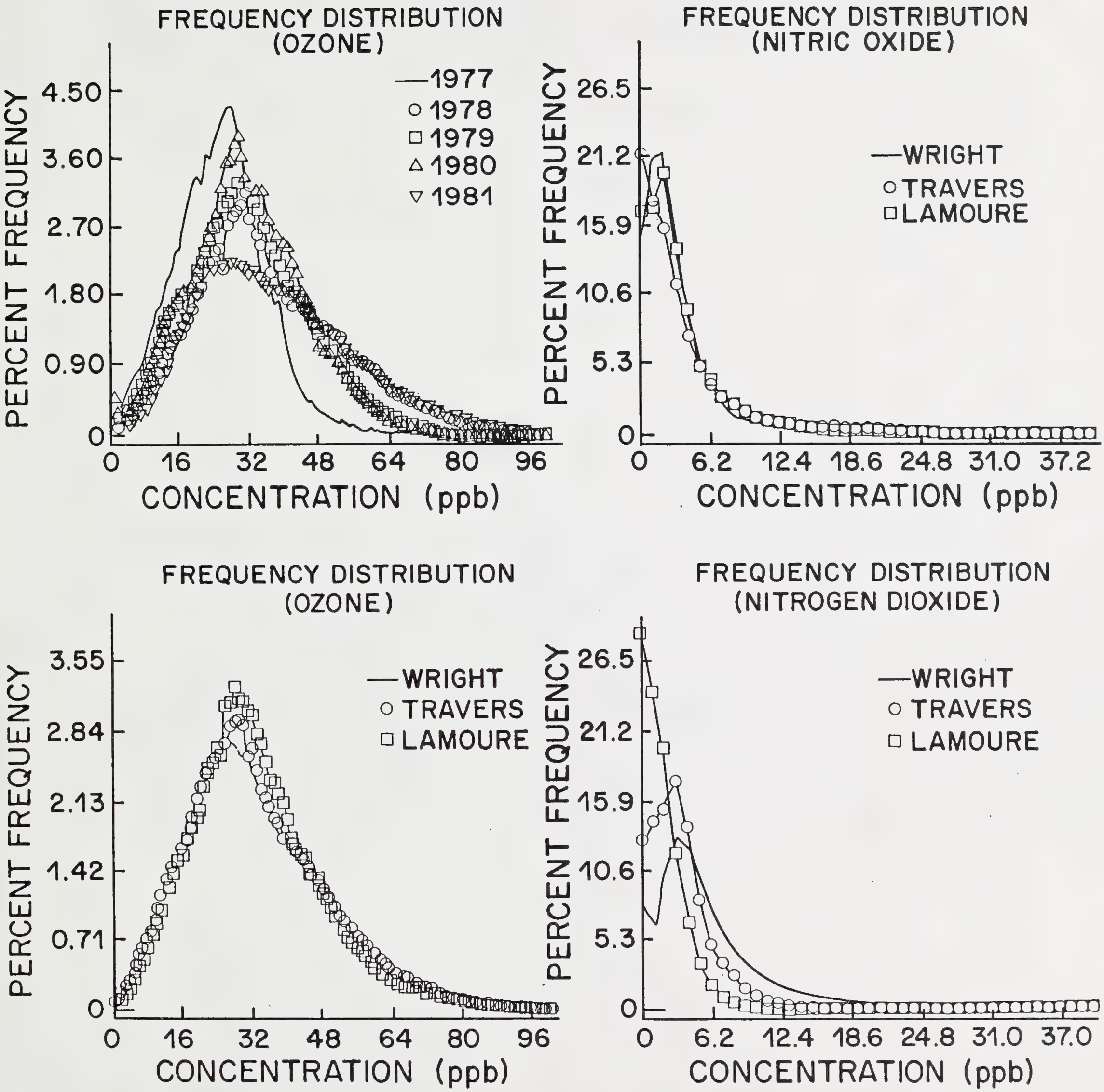

Figure 1. Frequency distributions for ambient ozone, nitric oxide, and nitrogen dioxide. In the upper left, the frequency distributions for ozone are broken down by years, whereas in the bottom left they are broken down by site. Only minor differences were observed among sites. Among years, 1978, and particularly 1980, had more high O_3 concentrations. The upper right shows the frequency distribution for nitric oxide broken down by site. The concentrations were similar at all three sites. The bottom right shows the frequency distribution for nitrogen dioxide broken down by site. Major differences in the concentrations of NO_2 occurred at the different sites, with a gradient extending out from the urban area. (from Pratt et al. 1983).

Table 1. Frequency distribution of averaged hourly SO_2 concentrations downwind from a large point source. Data from 7 air quality monitoring sites were examined in developing this summary statistic.

SO_2 Concentration (ppb)	Absolute Frequency	Relative Frequency (%)	Cumulative Frequency (%)
0	89,192	94.4	94.4
5	3,446	3.6	98.0
10	1,316	1.4	99.5
15	260	0.3	99.8
20	142	0.2	99.9
25	37	0.0	99.9
30	24	0.0	100.0
35	8	0.0	100.0
40	9	0.0	100.0
45	3	0.0	100.0
50	4	0.0	100.0
70	2	0.0	100.0
130	1	0.0	100.0

Source: Fowler and Cape (1982)

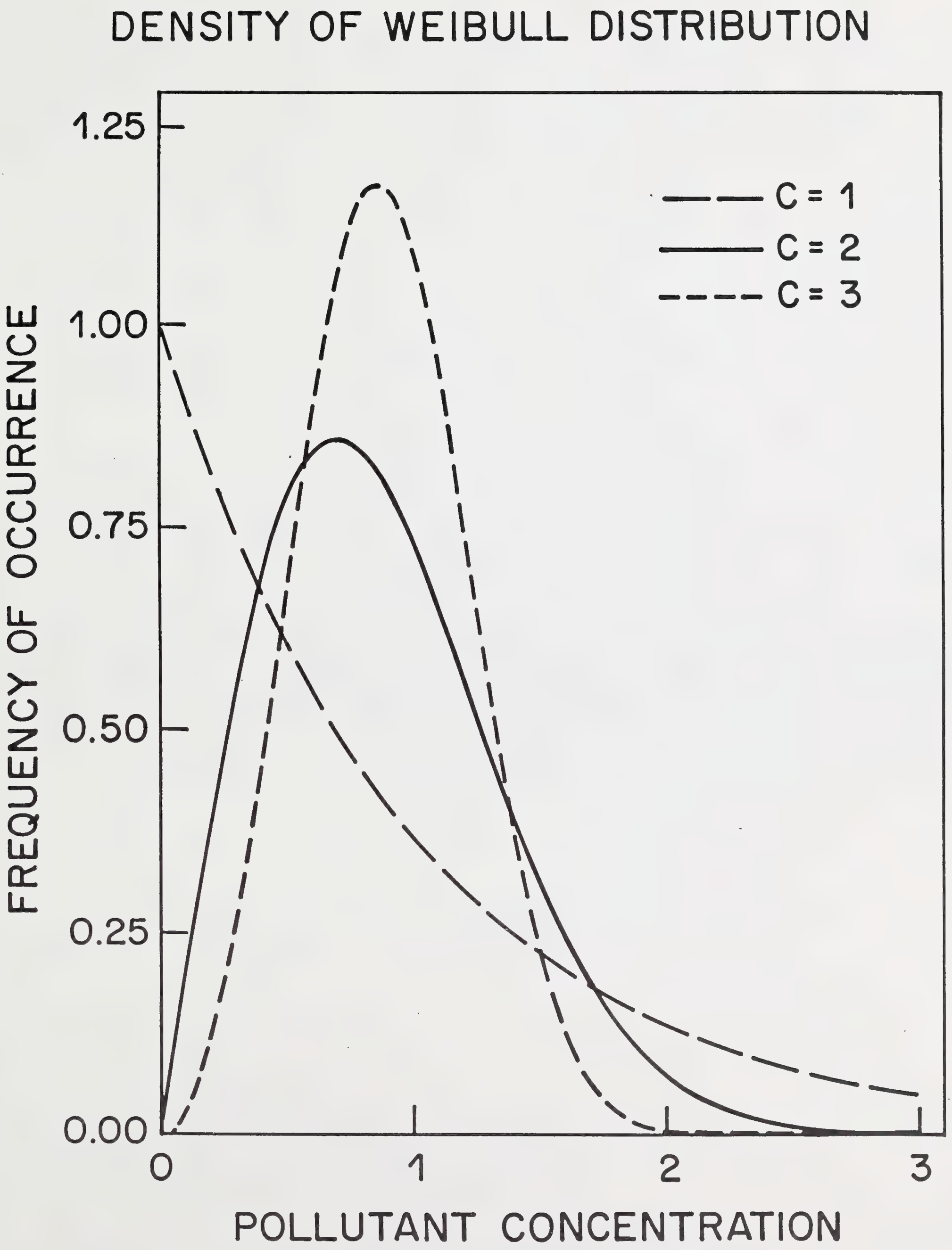

Figure 2. Theoretical distributions illustrating the Weibull family of frequency distributions.

In addition to the previous discussions on gaseous pollutants, the phenomenon of "acidic rain" is of major international, ecological concern. Our knowledge of the observed or potential effects of "simulated acidic rain" on crops and tree species have been summarized by Irving (1983) and Jacobson (1984). As far as we know there are no demonstrated cases of direct negative effects of "acidic rain" on vegetation under ambient conditions. Almost all studies relate to the use of "simulated rain". This consists of treating plant species with a "solution of constant chemical composition, applied artificially at constant or varying rates and amounts". In our opinion this is irrelevant to the real world where the chemistry of precipitation varies significantly within and between individual rain events (Pratt and Krupa 1985). The observed temporal and spatial variability of rainfall properties is regulated by: (a) regional versus local meteorology; (b) regional versus local distribution of pollutant sources and their characteristics; (c) the frequency of rainfall; (d) rainout versus washout; and (e) the concentration of coarse particles in the air prior to the rain event.

The literature contains numerous publications where "average" values of constituents in precipitation have been used to develop the "simulant" in plant exposure studies. As with the gaseous pollutants discussed previously, the frequency distributions of the concentrations of ions in precipitation also do not follow normal distribution. Such distributions are best described by a Weibull function (Nosal and Krupa 1986).

In describing the relationships of ions in precipitation, frequently linear, statistical regression methods are used. Such techniques assume that frequency distribution data is normally distributed, and the residuals are: (a) unbiased (mean zero); (b) homoscedastic (equal dispersion); (c) normal (Gaussian dispersion); and (d) independent. Recently, Nosal and Krupa (1986) showed that the aforementioned assumptions are violated by precipitation chemistry data (Tables 2-5). In addition, there are a number of other concerns introduced through artifacts caused by:

1. Sampling methodology (Coscio et al. 1982; Electric Power Research Institute 1986);
2. Sample collection period (event or daily versus weekly or monthly) (de Pena et al. 1985; Ridder et al. 1985; Sisterson et al. 1985; Krupa, unpublished); and
3. Methods of numerical analysis used in the data analysis.

Krupa (unpublished) found that:

1. There are significant differences in the chemistry of precipitation, as derived from numerical analysis, between warm (April 15 - October 14) and cool (October 15 - April 14) seasons. This is to be expected.
2. The concentrations of certain ions (e.g., SO_4, NH_4, Ca) are greater in the warm season compared to the cool season. This is also to be expected.
3. However, the cool season, rather than the warm season chemistry regulated the results of data analysis on an annual basis at many geographic locations in the US. In other words, results of statistical analysis of annual data resembles more closely the cool season, rather than the warm season chemistry.

Table 2. Summary statistics of the distributions of wetfall parameters.[a]

Location	Parameter	Coeff. Skewness[b]	Coeff. Kurtosis
Fernberg	pH	4.14	0.97
	$\log_{10} SO_4$	4.13	2.01
Marcell	pH	3.94	-0.05
	$\log_{10} SO_4$	2.20	1.30
Lamberton	pH	-2.63	-0.77
	$\log_{10} SO_4$	2.03	2.36
All Locations Pooled	pH	3.30	-3.47
	$\log_{10} SO_4$	4.07	2.03

a Data for the three Minnesota sites were gathered by the National Atmospheric Deposition Program (NADP 1978-1984), Natural Resources Ecology Laboratory, Colorado State University, Fort Collins, Colorado.

b Standardized test values, at 95% significance level, critical value for normalcy is $\pm$ 1.96 for skewness.

Table 3. Distribution of some major wetfall chemical components at Marcell, Minnesota.[a]

Distribution	Ion	Chi-Square	Significance	K - S[b]	Significance
Gamma	SO_4	82.551	1.58E-13	.1635	2.28E-6
Lognormal	SO_4	19.322	.013	.0434	.999
Weibull	SO_4	65.115	1.37E-10	.1126	3.01E-3
Gamma	NO_3	96.000	0.0	.1978	0.0
Lognormal	NO_3	13.135	.0688	.0566	.3863
Weibull	NO_3	60.659	3.46E-10	.1110	3.51E-3
Gamma	pH	23.941	.1210	.0688	.1550
Lognormal	pH	21.906	.14624	.0623	.2446
Weibull	pH	52.127	1.96E-5	.1007	8.36E-3

a Data were gathered by the National Atmospheric Deposition Program (NADP 1978-1984).

b Kolmogorov - Smirnov distance.

Table 4. Summary statistics of the multivariate regression to predict the relationship of log SO_4 with other chemical constituents in wetfall.[a]

Regression equation:

$$\log SO_4 = 1.44 + 0.307 \log Ca + 0.042 \log Mg + 0.346 \log NH_4 + 0.174 \log Na - 0.163\ pH$$

Variable	Coefficient	St. Dev.	T-ratio
Constant	1.4395	0.0545	26.42
log Ca	0.3067	0.0370	8.30
log Mg	0.0425	0.0350	1.21
log NH_4	0.3460	0.0183	18.93
log Na	0.1743	0.0154	11.31
pH	-0.1633	0.0109	-14.93

S = 0.1497; R^2 = 77.5%; R^2 adjusted for degrees of freedom = 77.3%

Analysis of Variance

	d.f.	SS	MS
Regression	5	42.9881	8.5976
Residual	558	12.5101	0.0224
TOTAL	563	55.4981	

[a] Minnesota data from the National Atmospheric Deposition Program (NADP)

Table 5. Summary statistics of the tests of normality of the residuals in Table 4.

Coefficient of skewness = 0.690941
Standard value = 6.6989
Root (skewness) = 2.588
Lower crit. (95%) = -0.179
Upper crit. (95%) = 0.179
Distribution of the residuals is significantly skewed to the right.

Coefficient of kurtosis = 7.57087
Standard value = 22.1581
Lower crit. (95%) = 2.67
Upper crit. (95%) = 3.37
Distribution of the residuals is significantly leptokurtic.

Chi-squared = 25.44 (12 degrees of freedom)
Significance of departure from normality = 0.012
Distribution of the residuals is significantly non-normal.

Durbin-Watson statistic DW = 1.66123
DW < DW upper (5%) = 1.78; reject rho = 0
Residuals are autocorrelated with respect to time; hence dependent.

Stratification of residuals by pH range - 4.8 - 5.1 - 6.2 -

Test of Homoscedasticity	Statistic	Significance
Cochran's C = Max. Var / Sum. Var.	0.3704	.0000
Bartlett - Box F	13.901	.0000
Bartlett	1.07755	.0000
Hartley's Max. Var. / Min. Var.	2.503	.0000

Distribution of the residuals is significantly heteroscedastic.

While it is not clearly described in a number of publications on the effects of simulated acidic rain on vegetation, we wonder how many scientists used annual statistics in designing their studies with "simulated rain". After all, plants achieve active or pollutant sensitive growth stages (e.g., soybean flowering and pod filling) only at certain times of the year.

Of particular concern is the definition of the time series of the occurrences of rainfall of sufficient intensity (rate and amount) and chemistry of concern, its relationship to the occurrence of other forms of pollutants, and the timing of such interactive pollutant stress in relation to the growth stage and sensitivity of the plant species. This aspect of concern is discussed in greater detail in the next section of this report.

As opposed to the long-term emphasis of research on the effects of gaseous air pollutants on plants, and the recent impetus to study the impacts of "acidic rain", little if any effort on a comparative basis has been directed to examine the effects of fine particles that contain a major fraction of SO_4, NO_3, etc. (Stevens et al. 1978). Many plant scientists have difficulty in addressing this question. Fine particles (< 1.5 μ) which are monodisperse and of uniform size and concentration are extremely difficult and complex to generate on a continuous basis. In addition to this problem, in our opinion, many plant scientists have not fully applied state-of-the-art atmospheric physics and chemistry in evaluating air pollutant - plant response relationships. Understanding the nature of the cause is as important as understanding the nature of the receptor response. In our opinion, sound integration of the two aspects is critical.

3. THE CONCEPT OF POLLUTANT DOSE

"Dose" is one of the most frequently used terms in air pollution - vegetation effects literature. "Dose" can be defined as the exact amount or extent of a given treatment to which a given receptor is subjected, at one time, or at stated intervals. The numerical expression of dose is an area of much controversy at this time.

Historically, dose has been expressed as ct - pollutant concentration, c, multiplied with duration of time, t, of exposure or as an average of pollutant concentration over exposure duration (c/t). More recently, it has also been expressed as "integrated exposure" (IE), as determined by summing the products of concentration times the exposure period, when the pollutant concentration exceeded a set, minimum threshold (Lefohn and Benedict 1982).

In the numerical definition of dose, several considerations are critical, in regard to both the cause (air pollutant) and the receptor (vegetation) response. Air pollutant averaging techniques assume normal distribution of ambient pollutant concentrations. However, as previously stated the distributions of ambient ozone (O_3) and sulphur dioxide (SO_2) concentrations are best described by Weibull and gamma functions (Berger et al. 1982; Lefohn and Benedict 1982; and Nosal 1984). A consequence of these non-normal distributions on the application of pollutant averaging techniques, for example, is illustrated by the work of Hogsett et al. (1985). In this study two exposure regimes were used to compare a set of episodic ozone exposure patterns with daily exposures. An episodic ozone pattern, applied to alfalfa over a 133 day growth period, elicited a greater growth response compared to a daily peak exposure pattern. The two profiles had similar integrated exposure values, but different 7-h season means. The 7-h (0900-1559 h) means for the two profiles were inversely correlated with the observed growth response. The episodic profile had a smaller seasonal mean, and yet caused a greater yield reduction.

Another example of the artifacts induced by pollutant averaging techniques pertains to sulphur dioxide concentrations downwind from a large point source in Minnesota (Krupa and Gardner, in preparation). Ambient ground level sulphur dioxide concentrations were monitored continuously over a 10 year period at seven locations relative to the source plume dispersion. When hourly pollutant averages were examined, SO_2 concentrations were reported to be zero during approximately 90% of the monitored period (Table 1). However, when the continuous data were examined, within the 90% time there were numerous instances when the plants were exposed to SO_2 concentrations as high as 0.50 ppm for five minutes. Even though in this particular case no negative effects were observed, it is important to note that it is well accepted that, with some exceptions, chronic effects are the result of the cumulative impact of intermittent episodes. Such a cumulative impact is not a straightforward additive function, because the final biological response is a product of the stress minus the ability of the plants to compensate (Zahn 1970). This brings forth the concept of frequency of occurrence of pollutant episodes and the time interval between such episodes. During the time interval between episodes, gaseous pollutants can and do exist in low concentrations. Exposure of plants to such low pollutant concentrations, can either predispose them to subsequent episodes or can confer tolerance (Godzik and Krupa 1982). These phenomena are confounded by the influence of other environmental variables and the biological time clock

(discussed in the following paragraph). Thus, in our opinion, under field conditions plants do not respond to a single pollutant exposure threshold value for injury, but a range of such values. Therefore, we believe that any single "cut-off" value as "threshold" makes little biological sense. It is a simplistic approach to our understanding of pollutant exposure - plant response relationships.

From the perspective of receptor (vegetation) response, plant physiologists and plant pathologists have clearly shown the importance of plant growth stage in the end response of vegetation to biotic or abiotic stress (Teng and Gaunt 1980; Benson et al. 1982). This introduces the concept of biological time clock and stress (Figure 3). For example, defoliation or foliar injury to soybean by hail during the early part of the plant's growth would have no effect on the final yield. On the other hand, such a stress during flower set to pod filling would result in significant yield loss (Lockwood et al. 1977).

In this context the influence of variables which regulate the rate of plant growth or its sensitivity to the pollutant stress is of great importance. Fundamentally the genetic characteristics of the plant species in question are a major factor. A number of investigators have shown that within a given crop species, under similar growing conditions, different cultivars of that crop respond differently to similar pollutant exposure regimes (Unsworth and Ormrod 1982). Because of the genetic variability or heterogeneity, natural or managed populations of trees also exhibit varied behaviour among individual trees within the population. This overall influence of the inherent genetic properties of the plant species is further confounded by the extraneous influence of atmospheric, edaphic, and additional biological variables.

Some atmospheric factors include light, temperature, relative humidity, and carbon dioxide. Edaphic factors such as moisture and nutrient availability concurrently regulate the overall plant growth and behaviour. The large temporal and spatial variability of all these factors is a major contributor to the uncertainty in regional scale crop loss estimates. These environmental factors not only regulate the rate of plant growth, but also many of them influence the stomatal behaviour. The stomata serve as the entrance in plants to atmospherically derived chemical energy (carbon). They also serve as the predominant pathway for the entrance of gaseous pollutants into the leaf. Majernik and Mansfield (1972) have shown that in bean plants stomata are opened and closed to varying degrees by the influence of the relative concentrations of carbon dioxide to SO_2. Similarly, plants subjected to temporary drought followed by the availability of sufficient moisture exhibit an increased sensitivity to O_3 exposures. Under ambient conditions such factors become even more complex with the influence of pollutant mixtures.

A number of investigators have developed crop loss models in evaluating the effects of pathogens and pests (Teng and Krupa 1980). In this field of research, many process-oriented models include the role of environmental variables. However, the influence of air pollutants has not been included in such models. Plant response to either the pathogens or pests and to air pollutants is influenced by interaction of these variables in a number of complex and yet to be fully understood ways [refer to Unsworth and Ormrod (1982)]. It is beyond the scope of this report to provide a detailed discussion of this subject.

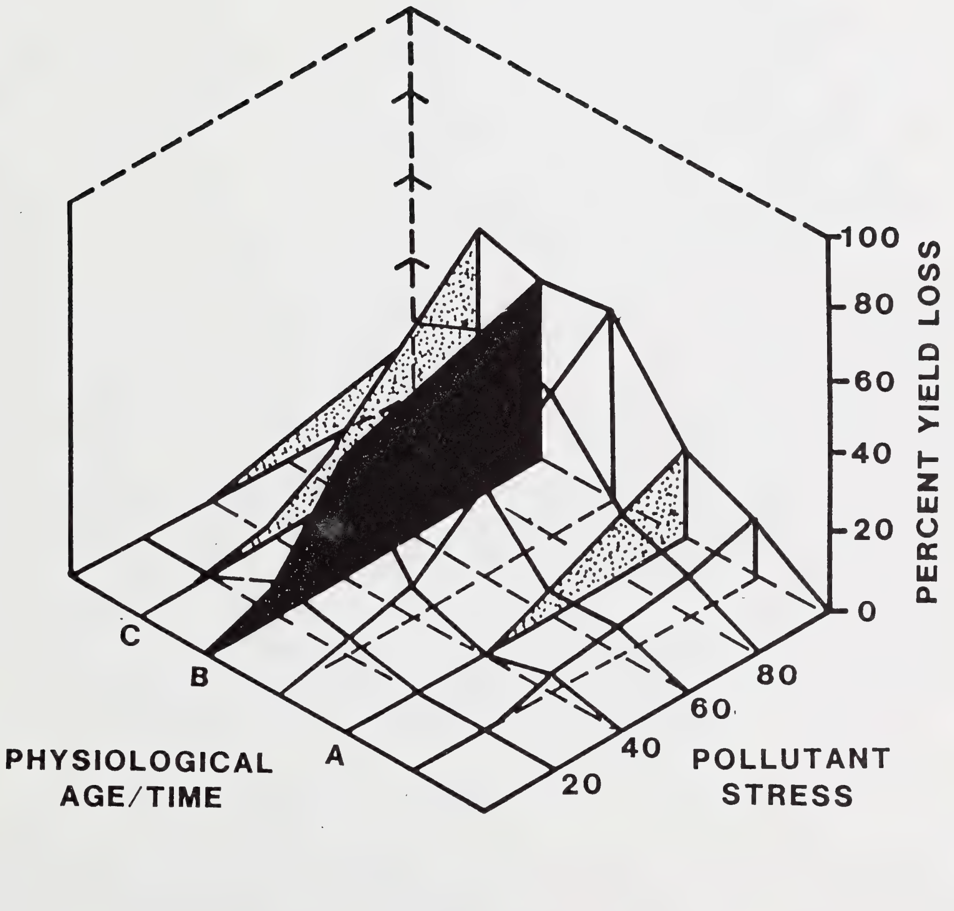

Figure 3. Conceptualization of the response surface of yield loss to pollutant stress as influenced by crop development stage.

In the context of air pollutant exposure and plant response, a satisfactory numerical expression of dose should at least consider, for example:

1. the artifacts of pollutant averaging techniques;
2. the episodicity of pollutant occurrence and exposure;
3. the time intervals between episodes; and
4. the relationship between the pollutant stress and the biological time clock (growth stage).

According to Runeckles and Brown (1986), one model which does not provide a simple dose statistic, but which minimizes the uncertainties of overall dose-response is that of Nosal (1983).

The model consists of a mixed, multivariate, polynomial, Fourier regression:

$$R = \sum_{i=1}^{3} \sum_{n} a_i^{(n)} x_i^n + \sum_{i=1}^{3} \sum_{m} b_i^{(m)} \sin \omega_m x_i$$

where:

R = plant response (crop yield parameters; annual basal area increment of trees, and so forth);

x_1 = number of pollutant episodes;

x_2 = cumulative integral of the pollutant episodes;

$\int_{t_2}^{t_1} c(t)\,dt$ = integral (exceeding 1) of the concentration and the duration of each episode, cumulative through the duration of the study ($t_1 - t_2$);

$c(t)$= pollutant concentration at time t;

x_3 = peak pollutant concentration, max $c(t)$ in ppb;

$t_1 < t < t_1$; and

$a_1(n)$, $b_1(m)$ = model parameters.

The model parameters are estimated using the least squares approach:

$$\min SSQ = (R - \sum_{i=1}^{3} \sum_{n} a_i^{(n)} x_i^n - \sum_{i=1}^{3} \sum_{m} b_i^{(m)} \sin\omega_m x_i)^2$$

The actual degree of the polynomial (range of the subscript "n" in the first double sum) and the number of sin terms (range of the subscript "m" in the second double sum) vary depending on the plant response type and the pollutant type. However, in general the polynomial degree $n \leq 2$ and sin degree $m \leq 1$ and $\omega_m = 1$ appear to be appropriate.

Thus, the model accounts for the number of pollutant episodes, highest peak pollutant concentration, and the cumulative numerical integral (concentration over time) of the exposure. The weakness of this model, however, is that it does not provide a complete numerical explanation of the importance of the individual episodes or its relationship to the biological time clock. However, it considers the concept of episodicity and fluctuations in ambient air quality over time with response, rather than attempting to define a single dose statistic.

While the previous narrative pertains to gaseous air pollutants, significant attention has been directed in recent years to the phenomenon of "acidic rain" (US National Research Council 1983). A number of investigators have used linear or linearizable statistical regression techniques in defining the temporal and spatial aspects of rainfall chemistry to which vegetation is exposed. Recently, Nosal and Krupa (1986) showed that the treatment of data by linear or linearizable regression methods violates the assumptions required for the use of such techniques (namely, normal distribution of data, normal distribution of the residuals in the regression, homoscedasticity, equal dispersion, unbias or mean zero, and independence). Such data also fail to qualify under "robust regression". These considerations are very critical, since almost all studies on the impact of acidic rain on vegetation relate to simulation experiments which are based on the assumptions found to be violated by Nosal and Krupa (1986).

This overall discussion points to the difficulties, artifacts, and errors associated with the numerical description of dose. Unfortunately, in the real world the vegetation is subjected to stress in a different manner. Any description of dose must make biological and statistical sense. If the two requirements can be achieved simultaneously, such an output would be a desirable solution to the problem.

One aspect of dose which has not been considered is the question of "exposure dose" versus "effective dose" (Runeckles 1974). Exposure dose may be defined as the pollutant regime to which the plant species is exposed as defined by appropriate ambient or atmospheric measurements. Effective dose may be defined as the actual quantity and rate of the pollutant which is absorbed by the plant. It is the "effective dose" that results in the observed or measured effect. However, since the numerical definition of "exposure dose" itself is an area of much controversy, no effort is made here to examine the details of "effective dose". In addition, at present we are not aware of techniques to accurately measure the "effective dose" under field conditions. Possible approaches include the use of tracers such as stable or radioactive isotopes. Such methods, however, are highly complex and are limited by the time of integration required to measure their changes in concentration within the plant tissue. Another approach is the computation of pollutant absorbed dose (PAD) as suggested by Fowler and Cape (1982). PAD = mean pollutant concentration ($\mu g/m^3$) x exposure time (s) x canopy conductance (m/s).

4. DEFINITION OF THE TYPES OF MODELS

An "empirical model" as used in the literature on the subject matter, has usually meant a mathematical equation that has been derived statistically from a set of data. According to Woodmansee (1974) a statistical model can be defined as "an equation in which the dependent variable is estimated by combining one or more independent variables each of which is multiplied by an appropriate coefficient, in various additive combinations". In contrast, a "mechanistic, process model" is defined by Woodmansee as "one which attempts to represent a biological system in terms of basic, well defined laws or relationships".

With regard to plant response, we frequently use simplified mathematical models of a few variables, usually describing how much of something exists, rather than at what rate it is changing. Usually the description consists of one equation, rather than a set of equations, as an empirical model. An example is the crop-weather model used for regional and inter-regional forecasting. At the field level, we believe that the empirical, statistical, "regional scale variable-based" models can suffer from a lack of realism and generality (ability to be applied in conditions outside of those for which it was developed). As a result we choose to emphasize in this review the other types of growth-production models which generally use a series of equations to describe rates of changes of various physical and biological processes, along with environmental constraints which can change those rates. Kercher and King (1985) also take a similar view.

A useful framework for viewing various plant growth, development and production models is one which is ecological in nature and refers to the resources that control or regulate rates of growth. This framework consists of four increasingly complex levels of production (de Wit and Penning de Vries 1982; Penning de Vries 1982a,b). Van Keulen and de Wit (1982) presented the same framework in the context of more comprehensive farming systems analysis and land use management.

Crops process models tend to be in one of the following categories:

Production level 1: Plant growth is limited only by light and heat (weather);

Production level 2: Plant growth is limited by shortage of water availability, during part of the time;

Production level 3: Plant growth is limited by nitrogen shortage, during part of the time;

Production level 4: Plant growth is limited by shortage of phosphorus and other needed minerals.

A production level which should be included is the "plant growth limited directly by industrial pollutants". Superimposed on all these would be models of the interactive effects of plant pathogens and pests. We know of only one review which covers the topic of models for studying the effects of toxic substances on crop growth (Kickert and Benenati, In Press). In addition, it is not clear to us the extent to which nutrient fertilizer - plant growth models include growth retarding effects caused by fertilizer overdose.

Table 6 provides a summary of the advantages and limitations of the two major classes of models (empirical and mechanistic) reviewed in this report.

Table 6. Advantages and limitations of the types of models.

Feature or Characteristic	Empirical Statistical Regression Models	Mechanistic Process Models: Preliminary Model	Mechanistic Process Models: Comprehensive Model	Mechanistic Process Models: Summary Model
Relative accessability of input requirements	High (+)[1]		Medium - Difficult (-)	
Amount of input data required to use/enter	Low (+)		Medium - High (-)	
"Simplicity"[2]	"High" (+)	"Medium"	"Low" (-)	"Medium"
Time required for computer to run	Low (+)		Medium[3]	
Amount of device memory required	Low (+)		Medium - High[3]	
Precision of responses (output)	High (+)[4]		Low - Medium (-)	
Ability to estimate response probabilities	High (+)		Low (-)[5]	
"Predictive value"	"Medium"	"Low" (-)	"Medium"	"High"
Realism	Low (-)		Medium - High (+)	
"Scientific value"	"Low" (-)	"High" (+)	"High" (+)	"Low"
Applicability to other locations (generality)	Low (-) (case history)	High (+)	Medium -	
Typical application (geographic area size)	Regional or local		Local	
"Instructive value"	"Low" (-)	"Medium"	"Low" (-)	"High"

[1] (+) is an Advantage; (-) is a Limitation.
[2] Quoted entries are from Penning de Vries (1983).
[3] Not very relevant if using 80286 microcomputers, or better.
[4] If no extrapolition outside the range of original database.
[5] Most of these models are deterministic, but could be modified by an experienced modelling specialist to run in a probabilistic mode.

5. MATHEMATICAL MODELS FOR CHARACTERIZING PLANT RESPONSE TO AIR POLLUTANT STRESS

Plant response can be defined as an observable or measurable change in the condition of a plant or a vegetation community due to the exposure to some air pollutant(s). As previously discussed, such responses can be classified as "acute" or "chronic". Independent of these two types, we are particularly interested in the final plant response that can be interpreted by natural resource and agricultural economists in cost-benefit assessment. Such an assessment is required in formulating and implementing policies relevant to air quality. In the present context there are two distinct steps involved in developing cost-benefit analysis:

1. Development and application of assessive and predictive models which will provide information on plant response to air pollutant stress; and
2. Development and application of economics models which can be applied to the information derived in step (1).

This report is restricted to a discussion of step (1), air pollutant exposure - plant response models. Tables 7A and 7B summarize the characteristics of selected empirical, regression models. A similar analysis is provided for the mechanistic, process models in Tables 8A and 8B. The actual mathematical equations relevant to models having sufficient documentation are presented in Appendices 8.1 and 8.2. The information contained in the Appendices can be applied to other appropriate situations by investigators other than the original authors.

This review identifies the advantages, limitations, applicability, and suggested modification of the models (Tables 7A and 7B; 8A and 8B). To some extent the properties described in these Tables are inherent to either class (empirical or mechanistic) of models (Table 6).

5.1 ACUTE POLLUTANT EXPOSURE AND PLANT RESPONSE

There are a number of models for describing acute pollutant exposure and subsequent plant response (O'Gara 1922; Thomas and Hill 1935; Zahn 1963; van Haut and Stratmann 1970; Larsen and Heck 1976; and Umbach and Davis 1986;).

Of the recent studies, Larsen and Heck (1976) presented a statistical model of acute response caused by O_3 and SO_2, in terms of visible injury symptoms on the leaves of a number of crops. Their equation (refer to the Appendices) is unusual, somewhat awkward to use for evaluating plant response, and is based solely on pollutant concentration and duration under optimal plant growth conditions. Umbach and Davis (1986) used essentially the same model in their studies.

Benson et al. (1982) provided a statistical model (refer to the Appendices) for acute response of alfalfa. While it is simple to use, it should only be used for very preliminary assessments, especially in locations outside Minnesota.

A statistical model for describing NO_2-induced acute injury was developed by Heck and Tingey (1979) (refer to the Appendices). As with most regression models used to describe the acute effects of air pollutants, it does not consider sub-optimal conditions, and therefore, should only be used with great caution for preliminary field assessments.

Table 7A. Empirical statistical models of air pollutant exposure - plant response.

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
1.	Nosal (1983)	Soybean chronic	SO_2; O_3	Number of pods per plant; seed weight per plant; number of seeds per plant; weight of 1000 seeds.	Number of pollutant episodes; cumulative concentration for duration of all episodes ppb; peak concentration (ppb).	None specified	Crop yield responses are assumed to be statistically associated with pollutant regime properties.	No development of independent field tests available for soybean.	R-square regression values given for various plant responses to various pollutant concentrations; all R-square > 0.85.
2.	Nosal (1984)	Northern coniferous forest chronic	SO_2	Annual basal area growth increment for lodgepole pine.	Same as above	None specified	Tree growth response is assumed to be statistically associated with pollant regime properties.	No development of independent field tests available for other forest plots.	R-square regression values given for five locations at varying distances from emission source.
3.	Fox et al. (1986)	Western larch chronic	SO_2	Annual tree trunk radial growth.	Smelter emissions of sulphur (t/y)	Precipitation	Tree ring width series away from the affected locations are assumed to represent macroclimate effects on annual tree ring growth. Deviations for trees near sulphur-emitting smelters are assumed to be caused by exposure to sulphur in the air.	Not applied independent of sites used to develop.	Some scattered evidence.

continued...

Table 7A (Continued).

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
4.	Stevens and Hazelton (1976)	Winter wheat; alfalfa acute and chronic	SO_2	Percent leaf area destroyed and percentage of yield.	Continuous, constant hourly average concentration (ppm) above thresholds for time durations.	None specified	In the absence of any other growth-limiting and susceptibility-reducing environmental constraints, crop yields are reduced when single or multiple periods of concentrations (exposure) exceed various effect-causing thresholds.	None	Tables of ranges of leaf area and yield responses are given by pollutant concentration and duration, but no quantitative sensitivity values are calculated; R-square regression values given for some of the equations.
5.	Rowe and Chestnut (1985)	Dry beans; cotton; grapes; potatoes chronic	SO_2; O_3	Per acre yield	Average hourly O_3 per month summed over growing season (pphm); number of growing season daylight hours when $O_3 \geq 10$ pphm; number of growing season daylight hours when $O_3 \geq 6$ pphm; number of growing season daylight hours when $SO_2 \geq 10$.	None specified	Some crop yields in the field change as a consequence of air pollution exposure.	Equations not independently tested, but crop sensitivities are compared to other studies with mixed results.	NA

continued...

Table 7A (Continued).

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
6.	Benson et al. (1982)	Alfalfa acute and chronic Corn; wheat; potatoes chronic	O_3	Loss in alfalfa foliar amd stem biomass weight; seasonal yield loss for corn in weight per 100 kernels; for wheat in weight per 100 seeds; and for potatoes in tuber weight.	Sum of hourly average concentration per day (ppb/day); accumulative sums of hourly average concentrations for weekly periods over the entire season (ppb/h).	None specified	Exposure to the pollutant results in uptake by the crop and is the sole cause of reduction in production of merchantable parts.	Applied state-wide; not field checked for validity of estimated losses.	R-square regression values: corn (0.876), potato (0.929), wheat (0.949), and alfalfa (0.131 to 0.999).
7.	Heagle et al. (1986)	Soybean chronic	O_3	Foliar injury percent; filled pod field density; filled pod weight; seed weight; 100 seed weight.	7-h daily seasonal mean (ppm).	None specified	Crop yield change is related to ozone concentration over the growing season but processes are not modelled.	Field data used for model definition only.	Standard errors for parameters are generally lower for Weibull model than polynomial forms.
8.	Heck et al. (1984a,b)	Wheat; barley; sorghum; corn; soybean; peanut; kidney bean; cotton; tomato chronic	O_3	Seasonal percent change in: wheat, sorghum, corn,soybean and kidney bean seed yield (kg/ha); barley seed weight per head; peanut pod weight per ha; cotton lint and seed weight per ha; tomato fresh weight per plot.	7-h daily seasonal mean concentration (ppm).	None specified	Crop yield change is related to ozone concentration over growing season; but processes describing how are not given.	Use exposure and crop yield field data (open top chambers) for model development; but not clear whether other data used to test models.	Relative yield losses for each crop at four seasonal 7-h daily mean ozone concentrations are given.

continued...

Table 7A (Continued).

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
9.	Heck et. al. (1982)	Soybean; lettuce; peanut; turnip; kidney bean. chronic	O_3	Dry weight of soybean seed/plant; fresh weight of lettuce head/plant; peanut pod weight/plant; edible turnip root fresh weight/plant; kidney bean dry weight/plant	7-h daily seasonal mean concentration (pphm).	None specified.	(Same as above).	Not tested independently to other locations.	R-square regression values for linear relations of yield to ozone range from 0.65 to 0.996; R-square values for plateau linear relations range from 0.94 to 0.99.
10.	Larsen and Heck (1976)	Various grains, vegetable crops; tobacco; ornamental plants and deciduous trees.	O_3; SO_2	Leaf injury symptoms.	Pollutant concentration (ppm); geometric mean pollutant concentration for 1 h (ppm).	None specified.	Different levels of pollutant concentration can compensate to produce similar levels of leaf injury.	Not tested independently in field.	Multiple correlation coefficients are given.
11.	Loehman and Wilkinson (1983)	Soybean; wheat; corn chronic	O_3	Crop yield per plant for corn and soybean; seed weight per plant for wheat.	7-h daily continuous concentration (ppm).	None specifield.	Exposure to pollutant results in uptake by the crop and is the sole cause of reduction in production of merchantable parts.	Not tested independently in field.	None

continued...

Table 7A (Continued).

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
12.	Oshima et al. (1976)	Alfalfa chronic	O_3	Average leaf weight to total plant weight; total plant weight.	Sum of hourly ozone average concentration above 10 pphm during daylight hours over entire growing season.	Average daily maximum and minimum temperature; average daily relative humidity.	Different seasonal doses of ozone are associated with changes in alfalfa foliar and whole plant production.	Yield reduction conversion function was compared to independent results and was found to correspond well.	t-values of regression coefficients are given for the four independent variables in various combinations.
13.	Westman (1979)	Coastal sage scrub chronic	Oxidants; hydrocarbons; NOx;CO; SO_2 particulate matter; oxidants + SO_2; NO_2 + SO_2.	Percent cover by native plant species.	Mean annual oxidant concentration (pphm).	Amount of litter; light; canopy height; longitude; latitude; distance to coast; elevation; slope; aspect; soil bulk density; soil texture; soil water field capacity; soil fertility; soil pH; mean, minimum, maximum temperatures of coldest and warmest months; annual precipitation; mean monthly precipitation of driest and wettest months; minimum time since last fire event; grazing history intensity,	Productivity and species composition differences of native sage scrub communities at various elevations are mainly associated with mean annual oxidant exposure; this spatial pattern might indicate a long-term process (change) that occurs over time in this region.	Conceptual model was tested by reciprocal average ordination of floristic variation and semi-log plot method for community composition comparisons. Results support the model.	Path coefficients and standard errors are given for path model fitted to data.

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Table 7A (Concluded).

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
14.	Medeiros et al. (1983)	Soybean chronic	Oxidants; acid precipitation.	Bushels of soybean per acre.	Hydrogen ion concentration in precipitation (moles/litre); 7-h daily mean oxidant concentration (pphm).	Heat (maturity zone); relative humidity.	Mixtures of pollutants and other environmental conditions affect crop yields.	Only applies to other field studies having one of the two exposure statistics; expected yield gains with control are 2x to 5x greater with only one pollutant.	Limited to field application results. (See column to left.)
15.	Heck and Tingey (1979)	Ornamental plants; vegetable crops; small grains; grass. acute	NO_2	Vegetable crops and grains: average of three most severely injured leaves of percent leaf area with chlorosis or necrosis; Ornamental plants: averages and injury percentage for entire plant.	Continuous constant concentration (ppm) for durations of 0.5 to 7 h.	None specified	Average percentage of leaf injury varies according to the exposure concentration and duration.	Not tested independently in the field.	Some crops showed no response up to 7 h with 20 ppm NO_2. "Intermediate" and "susceptible" crops have R-square regression values ranging from 0.31 to 0.83.

Table 7B. Empirical statistical models of air pollutant exposure and plant response - model description.

No.	Reference	Mathematical Nature: Exposure	Mathematical Nature: Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
1.	Nosal (1983)	Multivariate polynomial Fourier equation involving the three exposure properties.	First-order nonlinear polynomial regression equation for each plant response property.	IBM/XT	APL PLUS	Resulting regression equations with statistics given; program code not published; system flowchart not relevant to approach and not given.	More realistic representation of specific pollutant exposure conditions triggering plant response; high R-square regression values in polluted environments.	If used with a single plant response, without considering growth processes and other limits to growth, it offers little more insight on how plants respond than other statistical models.	Environmental assessment or research where a data-base for continuous pollutant monitoring is available along with plant growth observations.	Should be integrated into a process-oriented crop summary model. Needs more field testing.
2.	Nosal (1984)	Multivariate polynomial Fourier equation involving the three exposure properties.	First-order nonlinear polynomial regression equation for the plant response variable.	IBM/XT	APL PLUS	Same as above.	Same as above.	Same as above.	Same as above.	Should be integrated into one of the process models for forest such as SILVA. Needs more field testing.
3.	Fox et al. (1986)	Single multivariate linear regression equation with tree growth as a function of sulphur emission.		NA	NA	General form of single statistical regression equation only.	Simple. Relates former environmental conditions to current vegetation response.	No coefficient values given in publication. Need several years of data to use. Inadequate documentation. Exposure is implied by emissions only.	Approach could be tried for assessment elsewhere, but the specific model cannot be used because of inadequate documentation.	None

continued...

Table 7B (Continued).

No.	Reference	Mathematical Nature: Exposure	Mathematical Nature: Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
4.	Stevens and Hazelton (1976)	Linear time-concentration (above threshold) equations based on O'Gara (1922) and others.	Levels of leaf destruction determine threshold concentrations; linear regression equations for yield and leaf destruction.	NA	NA	All regression equations given.	Simple One of the few models of acute response.	Not field tested; circular reasoning in that effect (leaf area loss) determines threshold concentration to calculate effect; title is wrong-this is not a "simulation". Doesn't consider other nonpollutant limits to plant growth.	Preliminary theoretical guidelines if nothing else is available.	None.
5.	Rowe and Chestnut (1985)	Linear regression equations of dry bean yield and cotton yield as functions of average hourly O_3 per month summed over growing season, and potato yield as function of number of growing season daytime hours of O_3 above 10 pphm and of SO_2 above 10 pphm. Nonlinear regression equation of grape yield as function of number of growing season daytime hours of O_3 at or above 6 pphm.		NA	NA	Regression equations and coefficients given for the four most sensitive crops.	Simple and easy to use.	Exposure definition is too simplistic; not independently tested in other areas; doesn't consider other nonpollutant limits to plant growth.	Preliminary assessment of yield loss.	None.

continued...

Table 7B (Continued).

No.	Reference	Mathematical Nature: Exposure / Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
6.	Benson et al. (1982)	Single nonlinear polynomial equation for alfalfa. Single multivariate (weekly periods) linear equation for corn; wheat; potato.	NA	FORTRAN	Statistical equations given; no computer programs published.	Simple and easy to use.	Exposure definition is too simplistic; not independently tested in other areas; doesn't consider other nonpollutant limits to plant growth.	Preliminary assessment of yield loss.	None.
7.	Heagle et al. (1986)	Various forms of non-linear Weibull model and polynomial models are used.	NA	NA	Mathematical equations given with parameter values.	Simple and easy to use.	Exposure definition is too simplistic; not independently tested in other areas; doesn't consider other nonpollutant limits to plant growth.	Preliminary assessment of yield loss.	None.
8.	Heck et al. (1984a,b)	Nonlinear Weibull model used to relate observed crop yield to an ozone exposure statistic; relative yield change is computed by yield differences under background and elevated ozone concentration, divided by yield under background concentration.	NA	Requires statistical analysis program, but not specified.	Crop yield equation given with table of parameter values by crop, cultivar, date, and location (but applicability to other locations and years is open to question).	Simple and easy to use	Based on field chambers. Exposure definition is too simplistic; not independently tested in other areas; doesn't consider other nonpollutant limits to plant growth.	Preliminary assessment of yield loss.	None.

continued...

Table 7B (Continued).

No.	Reference	Mathematical Nature: Exposure / Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
9.	Heck et al. (1982)	For crop yield as a function of seasonal 7-h/day mean O_3 concentration: - a simple linear equation - plateau-linear equation Percent crop yield reduction is a linear function of exposure statistic exceeding background.	NA	NA	Tables of parameter values are given for all models and crops considered.	Simple and easy to use.	Based on field chambers. Exposure definition is too simplistic; not independently tested in other areas; doesn't consider other nonpollutant limits to plant growth.	Preliminary assessment of yield loss.	None.
10.	Larsen and Heck (1976)	Multivariate nonlinear equation expressed as type of power function.	NA	NA	Equation and table of parameter values by crop are given.	One of the few models of acute response.	Equation must be rearranged to estimate plant response, is not easy, and mathematically questionable. Awkward definition of exposure.	Preliminary evaluation for air quality standard setting.	None.
11.	Loehman and Wilkinson (1983)	Single linear equation for soybean yield reduction with cultivar-dependent rate; nonlinear quadratic equation for corn and wheat yield reduction.	NA	NA	Equations given for each crop	Simple and easy to use.	Limited to conditions and database in Indiana.	Preliminary assessment of yield loss.	None.
12.	Oshima et al. (1976)	Plant response variables for the season are regressed against cumulative daytime ozone dose over the season.	NA	NA	Gives all regression equations, coefficients, and goodness of fit statistics.	Simple and easy to use.	Exposure definition could be improved.	Prelimary assessment of yield loss.	Should be field tested in other geographic areas.

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Table 7B (Concluded).

No.	Reference	Mathematical Nature: Exposure	Mathematical Nature: Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
13.	Westman (1979)	Not specifically documented.		NA	NA	Structural path model diagram presented, but no mathematical equations.	Provides an example of using a method not found elsewhere in air pollution-plant effects work.	Questionable because of insufficient mathematical documentation of results. Exposure definition is too simplistic.	Not possible as published because of inadequate documentation.	None.
14.	Medeiros et al. (1983)	Linear and nonlinear regression equations for yield as a function of both hydrogen ion concentration and oxidant.		NA	NA	Equations given along with error statistics.	One of the few models for pollutant mixtures. Considers other limits to plant growth.	Exposure definition could be improved.	Preliminary assessment of crop loss.	Should be merged with the exposure approach of Nosal (1983, 1984).
15.	Heck and Tingey (1979)	Additive linear equations are developed by species and cultivar to show NO_2 concentration at which mean percent leaf injury will occur for a certain exposure time duration.		NA	NA	Regression equations are given with coefficient values by crop by crop and cultivar.	One of the few models for acute response.	With the exception of ornamental plants, the percentage of foliar injury is not sufficient response information to assess economic impact. Is based on continuous constant pollutant concentration which can be unrealistic of field exposures.	Preliminary assessment of concentrations for legal air quality standard setting.	Need relations between percent foliar injury and yield loss. Needs a realistic fluctuating pollutant exposure relationship.

Table 8A. Mechanistic process models of air pollutant exposure - plant response.

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
1.	Kercher (1980)	Sugarbeet and various annual crops. acute and chronic	SO_2;H_2S	Gross and net photosynthesis; foliage biomass; stem biomass; fruit biomass; root biomass.	Pollutant concentration in air, continuously (ppm).	Light; heat; CO_2; precipitation; wind.	Physiological model of crop photosynthesis, allocation to plant parts for growth and yield over season under air pollutant with a threshold effect on photosynthesis.	No independent field tests aside from data used to parameterize model.	Not comprehensive; only CO_2 uptake versus H_2S and CO_2 concentration in air.
2.	Coughenour (1981)	Western wheatgrass rangeland. chronic	SO_2	Forage biomass; forage nitrogen and sulphur content (quality).	Continuous, constant concentration (µg/cc).	Light; heat wind; moisture; available nitrogen and sulphur.	Detailed physiolocial processes of sulphur uptake by leaves and roots, and movement between plant parts.	Shoot sulphur for the season from the model closely matched field observations.	SO_2 deposition rate is sensitive to concentration; forage amount; and soil water content; forage S content is sensitive to change in long-term ambient SO_2 concentration.
3.	Heasley et al. (1981)	Shortgrass prairie chronic	SO_2	Live plant weight above ground; shoot sulphur content.	3-h average SO_2 concentration at US federal standard level (0.50 ppm)	Light; heat; precipitation; relative humidity; wind.	Carbon, nitrogen, sulphur cycling through ecosystem consisting of physical processes vegetation, soil, and ruminant animals.	Soil moisture, plant weight, and shoot sulphur content over two seasons showed match between predicted and observed.	Over 31 year period, elimination of SO_2 influence revealed low sensitivity of all ecosystem components; inorganic S pool is relatively more sensitive.

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Table 8A (Continued).

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
4.	Kercher et al. (1980) Kercher and Axelrod (1981)	Conifer forest chronic	SO_2	Growth and survival of trees by species; basal area of tree stems by species.	Two options: SO_2 averaged over season, or accumulated dose (ppm); log of accumulated dose from successive episodes.	Light; heat; moisture; stress based on evapotranspiration; fire.	Dominance of a tree species in community is a result of competition caused by changes in species-dependent growth rate of individuals.	Unknown for air pollution conditions; but performance appears realistic and reasonable under non-pollution conditions.	See Kercher and Axelrod (1984).
5.	Luxmoore (1980)	Oak-hickory deciduous forest acute and chronic	SO_2; Zn; Pb	Plant tissue growth effect related to tissue pollutant concentration (accumulation).	Pollutant concentration in air (μg/mL); foliar uptake of particle deposition (g/m^2 land); foliar uptake of gases by diffusion, controlled by resistances (μg/mL).	CO_2; light; moisture.	Part of 5 complex interrelated models of carbon flow; biomass accumulation and transfer; water flow and soil chemistry-solute flow through plant physiological processes.	Applied to a field situation but not compared to independent field data.	Selectively; not comprehensive.
6.	King et al. (1983)	Soybean chronic	O_3	Soybean yield intended, but only ozone uptake is given in paper.	Mean hourly ozone concentration (pphm).	Light; heat; soil water potential.	Environmental factors control stomatal opening, which controls internal dose and affects photosynthesis, allocation of photosynthate to, and consequent seasonal yield of, plant parts.	None reported in this initial paper.	Daily ozone uptake versus soil water potential; light; temperature.

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Table 8A (Continued).

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
7.	King (1986)	Soybean chronic	O_3	Fraction of potential total plant yield.	Mean hourly ozone concentration (µL/L).	Soil water.	The ozone effect on relative crop yield depends on cumulative effect of ozone above a threshold and soil water available; effect depends on crop transpiration efficiency and actual transpiration.	Has not been field tested but author "illustrates range of model responses" by applying data for 24 locations in midwestern USA.	Biggest changes in relation between yield, drought, and ozone are associated with soil water content where moisture becomes limiting; and with sensitivity of transpiration to ozone dose.
8.	Miller et al. (1982)	Western mixed conifer forest chronic	O_3	Tree photosynthesis; tree foliar biomass; foliar litterfall; tree diameter growth; tree mortality; cone/seed production; seedling survival; forest tree species composition; dead tree fuel load.	Hourly average ozone concentration (pphm-h)	Heat; moisture; tree diseases; insect pests.	Photosynthesis of pines; population dynamics of trees as affected by physical growth resources; ozone; disease and insects.	Not able to do; mathematical models not completed.	Not able to do; mathematical models not completed.
9.	Ares (1979)	Coastal desert shrub steppe chronic	F	Carbon in leaves; fluoride in leaves.	Average daily ambient fluoride concentration (mg/m³).	Light; heat; rain; wind.	Mass balance of fluoride in vegetation and soil over growing season.	Development not yet to this stage.	Development not yet to this stage.

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Table 8A (Continued).

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
10.	Mortensen (1984)	Winter and spring cereals; legume crops; potato; sugar-beet; fodder beet; oil seed crops; grass; vegetables. chronic	SO_4; NO_3; Cd; Ca; K; Mg; Na; NH_4.	Ion concentration in harvested crop; pH in upper soil under crop.	Pollution concentration in air (µg/m³); deposition (annual) (for parent and daughter products) (g/m²).	None; growth is constant by month and crop type.	Mainly a soil chemistry budget model where crops are sinks for various ions in transit.	Not yet available.	Limited preliminary results in Christensen et al. (1985) for pH and cadmium in soil.
11.	Harwell and Weinstein (1983)	Eastern deciduous forest chronic	SO_2; O_3; NO_x	Annual productivity of forest stand.	Average annual pollutant load.	Light; heat; moisture; nutrients.	Individual tree growth in a stand is determined by physical resources needed; (after Weinstein 1982; Shugart and West 1977; and Botkin et al. 1972).	Development not yet to this stage.	Development not yet to this stage.
12.	Harwell and Weinstein (1983)	Eastern deciduous forest acute	SO_2; O_3; NOx	Percent change in fixed carbon partitioning; annual diameter growth.	Mean daily pollutant concentration.	Light; heat; moisture; nutrients.	Hourly, daily photosynthesis simulation (details not documented).	Development not yet to this stage.	Development not yet to this stage.
13.	Andersson et al. (1980)	Scots pine forest chronic	Acid precipitation	Annual wood production and nitrogen content.	Nitrogen as wet deposition (kg N/ha/y).	None specified.	Assumes acid deposition alters processes of N transformation in N cycle and tree growth changes as a result.	Development not yet to this stage.	Annual wood production is more sensitive to precipitation of N than to other N cycling processes.

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Table 8A (Concluded).

No.	Reference	Vegetation/Plant Timeframe	Air Pollutant(s)	Plant Production Response Properties	Air Pollutant Exposure Properties	Other Limits to Growth	Main Biological Paradigm	Field Application Results	Sensitivity Analysis Results
14.	Haines and Waide (1980)	Eastern deciduous forest chronic	Acid precipitation	Nitrogen in tree stems.	Constant pH of rain for 1h/week.	None described.	Mass balance N budget for hardwood trees; herbivores;woody litter; soil; soil microbiota; and meteorological wet and dry deposition.	Static budget model not suitable for field application except for location where developed.	Not available.
15.	West et al. (1980)	Eastern deciduous forest chronic	Not explicitly used.	Total tree biomass by species.	Not explicitly modelled.	Light; heat; soil litter.	Diameter and height growth of single trees among a mix of species each competing for different resource requirements for growth.	A prior version of the model was compared with/without American chestnut to historical records.	Total biomass by tree species in mixed species forest can be more or less than growth rate reduction; implying competition effects.

Table 8B. Mechanistic process models of air pollutant exposure and plant response - model description.

No.	Reference	Mathematical Nature: Exposure	Mathematical Nature: Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
1.	Kercher (1980)	"Instantaneous" concentration of gaseous pollutant in linear and nonlinear diffusion equations according to concentration and plant's threshold.	Net photosynthesis is depressed linearly above threshold, and increased quadratically below threshold in foliar diffusion.	NA	NA	System flow chart and mathematical equations are in Kercher (1978); program code not published.	Fairly realistic treatment of the plant physiological processes provides a useful tool for further in-depth research.	A number of difficult to determine parameters; numerical integration of "stiff" differential equations (with greatly differing time rates) requires a rare computer program; might be difficult to fully implement elsewhere.	Not applicable for operational use by other institutions for environmental assessment without considerable further research and development.	Pollutant exposure and uptake functions need further research and development.
2.	Coughenour (1981)	Linear equation for concentration diffusion resistance flow rate modified by leaf area index into leaves; root uptake of sulphate as Michaelis-Menton kinematics.	Sulphur transferred to plant parts by seasonal changes in shoot:root ratio for S/C.	NA	SIMPCOMP	System flow-chart and mathematical equations for biological and environmental processes, but no computer code published.	Incorporates several limits to plant growth and enables tracking of sulphur through ecosystem. Good field test results.	Constant, continuous exposure is unreal. Only provides bioaccumulation and whole biomass responses, not individual ecological effects.	Could be used to derive summary model(s) for the assessment of sulphur sinks.	Adaptation to annual small grain crops (for seed yield) would require careful examination of most mathematical equations. Exposure function needs to be changed to fluctuating, discontinuous inputs.

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Table 8B (Continued).

No.	Reference	Mathematical Nature: Exposure	Mathematical Nature: Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
3.	Heasley et al. (1981)	Steady state Gaussian plume model used to generate 3 h average SO_2 concentrations.	SO_2 deposition in canopy by diffusion resistance flow into foliage; finite difference equations for flows of C, N, S through ecosystem.	NA	FORTRAN	Gives system flowchart, but no mathematical equations for model.	Includes ruminant animals in the system. Good field test results.	Constant, continuous exposure is unreal. Only provides bioaccumulation and whole biomass responses, not individual ecological effects.	Not applicable because of inadequate documentation.	If mathematical documentation were available, the exposure submodel would need to be made more realistic.
4.	Kercher et al. (1980) Kercher and Axelrod (1981)	Simple seasonal average (accumulated dose) or episodal accumulations only.	Tree growth effect is patterned after empirical dose-response method of Larsen and Heck (1976).	NA	FORTRAN	Computer flowchart in Kercher and Axelrod (1984). Complete description in Axelrod and Kercher (1981)	Builds upon a well-used and respected tree growth and succession model. Includes climatic limits on tree growth. Complete documentation available.	Pollutant exposure mechanism and tree growth effect are not realistic. Not field tested under air pollution exposure yet.	Good for research, but with the right modifications and field testing, could be useful for assessment.	Pollutant exposure definition should be replaced with fluctuating, episodic function such as that of Nosal (1983, 1984).
5.	Luxmoore (1980)	Nonlinear gaseous diffusion equation for foliar uptake and cuticular conduction of the consituents of particulate matter.	Simple generic ramp function used to relate growth effect to tissue elemental concentration.	NA	NA	See Luxmoore et al. (1978) for general system flowchart; computer programs not published; complete mathematics not published.	Based on many realistic physiological processes.	Complete mathematics apparently not published; insufficient field testing. Might be difficult to implement on other computers.	Comprehensive model for research.	Biggest need is for complete documentation and field test of results.

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Table 8B (Continued).

No.	Reference	Mathematical Nature: Exposure	Mathematical Nature: Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
6.	King et al. (1983)	Accumulated ozone gas diffusion into foliage over a day.	Photosynthesis and ozone uptake respond to diurnal temperature and moisture stress in a complex set of equations.	NA	FORTRAN	NA	One of very few crop-oriented process models for pollution effects.	The only documentation is one preliminary paper; funding was terminated. Needs better air quality exposure definition.	General guide for researchers only.	Inadequate documentation prevents determining suggested modification.
7.	King (1986)	Ozone uptake is a power function of transpiration. Ozone dose is a power function of ozone damage reduction factor (transpiration ratio) times ozone concentration above a threshold.	Transpiration efficiency under drought and ozone is a non-linear power function of ratios of seasonal transpiration with and without ozone. Relative crop yield is determined as a simple product of seasonal transpiration ratios and efficiency ratios with, and without, ozone or soil water limits.	NA	NA	Eleven mathematical statements given in publication. No flowchart; no computer program.	Incorporates realistic field conditions of limited moisture for plant growth as an interaction with pollutant effects. Relatively simple model structure.	Not field tested. Structure is only for yield of entire plant, not merchantable plant parts. Uses questionable concept for duration and concentration of pollutant as daytime (only) dose. Does not use frequency or episodicity of exposure.	Very general preliminary guide on a regional scale where soil water, soil survey, and pollutant data are available.	Pollutant exposure concept should be modified to use concentration, frequency, and duration within a more realistic mathematical structure.

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Table 8B (Continued).

No.	Reference	Mathematical Nature: Exposure	Mathematical Nature: Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
8.	Miller et al. (1982)	Not able to do; project terminated prior to completion.	See Harwell and Weinstein (1983)	NA	NA	See references in Miller et al. (1982); system flowchart; some submodels have mathematics documented.	Comprehensive ecosystem view of the forest under air pollution stress. Considers effects of a variety of plant-injuring pests.	Inadequate definition of air quality exposure. Mathematical models and programs not completed.	General framework on how to design integrated forest ecosystem research and assessment programs.	Framework should have more emphasis on the single tree as a system, as well as the forest community.
9.	Ares (1979)	No mathematical equations given for this.	No mathematical equations given for this.	NA	NA	System flowchart and word model description only.	Provides example of a pollutant cycling system in semi-arid, sparse vegetation ecosystem.	Inadequate mathematical documentation. Mass balance approach only, no ecological effects per se.	General research framework.	Inadequate documentation prevents determining suggested modification.
10.	Mortensen (1984)	Root uptake proportional to water uptake and ion concentration in interstitial water on a monthly basis. Uptake from air from dry and wet deposition is a nonlinear equation; uptake proportional to total deposition and vegetation interception fraction.	Nonlinear algebraic equations for biomass, ion uptake, flows, and ion concentrations in crops.	B7800	FORTRAN	Mathematical equations and tables of coefficients; sample printouts in Christensen et al. (1985); program code not published.	Relatively simple. Considers a variety of compounds and elements associated with dry and wet acidic deposition.	Mass balance approach only, no ecological effects per se. Might be too simplistic to be useful for assessment. Preliminary version not yet field tested.	General preliminary guidance for research.	Needs functions for effects of tissue bioaccumulation on production and yield.

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Table 8B (Continued).

No.	Reference	Mathematical Nature: Exposure	Mathematical Nature: Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
11.	Harwell and Weinstein (1983)	Selected by probability from a historical frequency distribution.	Individual tree diameter growth is a second order function of maximum diameter and height for the species multiplicatively altered by availability of resources for growth.	NA	NA	NA	Based on the same well-respected predecessor model as that of Kercher and Axelrod (1981).	Exposure definitions are not adequate. Not sufficiently developed.	Not applicable due to inadequate documentation and early state of development.	Inadequate documentation prevents determining suggested modification.
12.	Harwell and Weinstein (1983)	No description for how the annual pollutant load is obtained from frequency distributions of mean daily concentrations.	Not documented.	NA	NA	Only an incomplete preliminary design paper was available for this review; no flowcharts.	Based on the same well-respected predecessor model as that of Kercher and Axelrod (1981).	Exposure definitions are not adequate. Not sufficiently developed.	Not applicable due to inadequate documentation and early state of development.	Inadequate documentation prevents determining suggested modification.
13.	Andersson et al. (1980)	Not explicitly modelled.	All N flows are linear equations.	NA	NA	System flowchart and parameter values given; equations can be constructed from these.	Relatively small and simple nitrogen cycle model.	As an acid deposition model, the definition of pollutant exposure is very incomplete. Vegetation growth only limited by nitrogen. No field test results.	Research only; not for assessment.	None. Other more comprehensive forest nitrogen cycling models exist that could be used.

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Table 8B (Concluded).

No.	Reference	Mathematical Nature: Exposure	Mathematical Nature: Plant Response	Computer Memory	Computer Language	Model Documentation	Advantages	Limitations	Applicability	Suggested Modifications
14.	Haines and Waide (1980)	Entered as increased ammonia N and nitrate N into the system from precipitation.	Root nitrogen content is a function of ammonia and nitrate N uptake as linear finite difference equations.	NA	NA	System flowcharts in Mithell et al. (1975); set of finite difference equations not shown but can be written from flowchart; computer code not published.	Relatively small and simple nitrogen cycle model.	Model documentation not clear or thorough. As an acid deposition model, the definition of pollutant exposure is very incomplete. Vegetation growth only limited by nitrogen.	Research only; not for assessment.	None. Other more comprehensive forest nitrogen cycling models exist that could be used.
15.	West et al. (1980)	Not explicitly modelled.	Tree species' sensitivities to visible leaf injury used to set constant loss of growth of either 0, 10, 20% in nonlinear difference equations.	IBM mainframe	FORTRAN	Computer program flowchart and mathematics in Shugart and West (1977); computer program in Botkin et al. (1970).	Provides indication of very long-term forest changes due to shift in balance of competition between species. Based on the same well-respected predecessor model as that of Kercher and Axelrod (1981).	Tree growth effect is assumed to be correlated with sensitivity to show visible foliar injury; a questionable relationship. No explicit exposure mechanism.	Research only; not for assessment.	Where it exists by tree species, growth decrease should be based on pollutant exposure, not visible foliar injury.

As with the three regression models described previously, in this report we refer to only three process-oriented models for acute response. Kercher (1980) described a comprehensive plant physiological model. However, the model requires improvement in describing the pollutant exposure kinetics. At this time it can be considered for research purposes only.

Harwell and Weinstein (1983) presented a preliminary paper for the design of a forest model capable of displaying acute effects. Attempts to obtain updated information from either of the authors were unsuccessful. At present it cannot be used in other assessment programs.

Luxmoore (1980) described an elaborate set of process models at the Oak Ridge National Laboratory (ORNL). This model is useful for evaluating acute effects in eastern deciduous forests relative to bioaccumulation of sulphur and heavy metals. Other air pollution research programs, especially those addressing local point source emissions of these pollutants, should investigate the accessibility of the documentation for this set of models. To our knowledge, the required documentation has not been published.

5.2 CHRONIC POLLUTANT EXPOSURE AND PLANT RESPONSE

Many models have been published to describe plant response to chronic pollutant exposure. Empirical, regression models for crops include those of Oshima et al. (1976); Stevens and Hazelton (1976); Benson et al. (1982); Heck et al. (1982, 1984a,b); Loehman and Wilkinson (1983); Medeiros et al. (1983); Nosal (1983); Rowe and Chestnut (1985); and Heagle et al. (1986). Appropriate information on any particular model can be obtained by crop type from Tables 7A and 7B.

For forests, only the statistical models of Nosal (1984), and Fox et al. (1986) were found to be sufficiently described that they could be considered for replication elsewhere. Clearly, the Nosal approach provides better results, probably because of a more realistic definition of the pollutant exposure.

In the last few years, a number of mechanistic, process-oriented and ecosystem level models have been published to analyse response of vegetation to chronic exposure to air pollutants. Some of these relate to crop responses (Kercher 1980; King et al. 1983; Mortensen 1984; and King 1986). The model of King (1986) is rather simple and easy to understand, but is in its early stages of development. It has a few limitations (refer to Tables 8A and 8B) which need to be rectified to make it useful for assessment.

There are also a number of process-oriented models developed for forests, rangelands, and desert shrub land exposed to pollutant stress. These include: Andersson et al. (1980); Haines and Waide (1980); Kercher et al. (1980); Luxmoore (1980); West et al. (1980); Coughenour (1981); and Heasley et al. (1981). Kercher and Axelrod (1984) provided a relatively realistic and especially well documented treatment that should be used as a foundation on which to improve our knowledge of forest assessment. However, as with most other models, it requires a more realistic mathematical definition of pollutant exposure in terms of frequency (episodicity), duration, and concentration of the pollutant(s).

For semi-arid rangelands, Coughenour's (1981) comprehensive model is well designed and documented (refer to the Appendices).

6. DISCUSSION AND RECOMMENDATIONS

6.1 REGIONAL SCALE APPLICATIONS

The use and applications of models at the regional scale can be separately considered for photochemical oxidants and for wet and dry acidic or acidifying pollutants.

However, there are a number of uncertainties attached to the assessment of air pollutant-induced ecological effects. Uncertainty is an accepted phenomenon when modelling biological systems. In the present context, "this uncertainty arises from the stochastic nature of many biological stimulus-response relationships and is a reflection of the inherent stochasticity of both the biological system itself and the environment that drives that system . . . (this) makes it almost impossible to predict a response that is deterministic, i.e., without variation (Krupa and Teng 1982).

Within the context of actual investigation, uncertainties originate from errors in: (a) monitoring the air quality; (b) experimental and numerical definition of pollutant exposure kinetics; (c) experimental design to characterize the cause and effects relationships; and (d) modelling the pollutant-response relationships.

Further, any transfer of results from unit level models to regional level leads to "scaling error". At present there is no general agreement among researchers on how to deal with the scale problem.

6.1.1 Air Quality Models for Photochemical Oxidants

There are a number of problems that must be considered in applying air quality models at the regional scale. The unavailability of air quality data at remote rural sites is one problem. The limitations of "averaging" air quality data (such as the popular 7-h daily average) also presents a problem in that, while it is simple, as discussed previously, it is unrealistic. An alternative to simple averaging is the three-parameter exposure kinetics described by Nosal (1983, 1984). Given the sparsity of rural oxidant data, the three parameters of exposure can be estimated for sites in a limited geographic region using the "Krieging" process of spatial interpolation (Lajaunie 1984). However, extreme caution should be used in applying this process, particularly if the number of actual data points in the interpolation is very limited.

There are also a number of assumptions made in the use of "Krieging". Such assumptions need to be tested at the outset, before the procedure can be applied to develop geographic predictions of photochemical oxidants.

6.1.2 Photochemical Oxidants and Regional Scale Plant Response Modelling

At least in the US, many believe that regional scale applications and air quality standard setting require a rather simple, one-independent-variable, single equation model. This model is best defined on the basis of statistical analysis of field data collected just for this purpose. A number of regression models discussed in Tables 7A and 7B were developed with this view. These models appear to provide high values of the coefficient of determination (R^2) because of the use of data sets of small sample size.

A group of counterpart scientists regard the mechanistic, process-oriented, or ecosystem models as suitable only for local site or point source applications. We agree

with this if one were thinking only of comprehensive models as described by Penning de Vries (1982b, 1983).

A number of scientists outside the US, and not in the field of air pollution - vegetation effects research, have argued that the way to obtain a simple, single (or few) equation(s) "summary model", possibly for regional scale applications, is to start with a "comprehensive" computer simulation of the biology (all the relevant components and processes, as they are known to function). Presumably, this model would be subjected to field testing, improved if needed, and re-tested. Then, it is used to derive the "summary model" equation(s), from the behaviour and sensitivity analysis of variables in the comprehensive model (Holling 1978; Penning de Vries 1982b, 1983). This is the approach that we recommend.

In addition to those process models reviewed in Tables 8A and 8B, there are quite a number of preliminary and comprehensive process models of crops and tree species not yet adapted to application in air pollutant - vegetation response research (Kickert 1984a).

To apply this strategy, one must evaluate the results of sensitivity analysis on the comprehensive process models to derive one or more summary models. The process models for O_3 effects (Tables 8A and 8B) on crops and tree species are not sufficiently complete to allow their use in the approach described here. As a result, summary models for O_3 exposure and plant response might be derived from:

1. Using the aforementioned strategy on the appropriate comprehensive models of SO_2 effects (Tables 8A and 8B) "retrofitted" for O_3 exposure and response; or
2. Using available non-pollutant summary crop models and adapting them to respond to O_3 exposure, through further research; or
3. Using available non-pollutant comprehensive crop models with aforementioned strategy for deriving summary models, and then adapting those models to O_3 exposure.

In each of these cases, we also recommend that the summary models be structured in terms of the probabilities of responses derived from probability density functions of the input parameters and forcing functions. This would enable the eventual users of these tools to judge the risks they choose to take in managing control technologies and strategies in their efforts to protect against initiating deleterious responses in vegetation.

Option (1) is recommended for obtaining a regional photochemical oxidant - forest response summary model, by starting with the SILVA model (Kercher and Axelrod 1981). In this effort, the SO_2 pollutant exposure sub-models could be replaced with a three-parameter (Nosal 1983, 1984) exposure model for oxidants. One or more summary models should then be derived and applied on a regional basis using "Krieging" (with strict regulations) to obtain the required input data.

For option (2), there is a published summary model called "SUCROS" for small grains including wheat (van Keulen and de Wit 1982) which includes phenological events (growth stages). This model could be used for Alberta. However, this model would also

need to be adapted for O_3 exposures. For regional scale applications, we recommend, with the restrictions described previously, Krieging, three-parameter exposure kinetics, and the input data for the "SUCROS" summary model.

For option (3), from the evidence provided by Kickert (1984b) for the sensitivity analysis of results of some crop models, the most sensitive factors (Kickert, unpublished) could be used to derive simplified summary models, for example, from the CORNGRO (corn growth) model. It must be realized, however, that: (a) the kinds of crops for which sensitivity data were described by Kickert (1984b) are far fewer than the number of different crops for which published, comprehensive process models exist (there are few or no sensitivity analysis data for wheat, barley, oats or alfalfa models, although such models are amenable to more sensitivity analysis - computer simulation experiments); and (b) corn is not a dominant crop in Alberta, Canada.

If existing models of small grains and alfalfa were to be used, then they would first have to be enhanced to respond to inputs of ozone exposure data, and sensitivity analyses would then have to be performed. For analysing potential crop response to regional scale pollutant exposure, this type of crop plant phenological model would then have to be reduced to a phenology-based summary model which would still contain a conceptual foundation based on processes (rather than being solely statistical, as are many dose-response models).

With any of these approaches, a hybridization between comprehensive mechanistic process models of crops and forest trees, and more simplified summary models could be obtained. Such models would be capable of responding to pollutant inputs on a regional scale and for rural areas, in ways that would be more meaningful than collecting a lot of field data and using routine statistical regression methods only.

In any of these options, for regional scale application, we recommend that researchers consider using the Krieging method in the strictest sense to derive data for three or four input parameters needed for a Mixed Multivariate Polynomial - Fourier type exposure model. Such information should be coupled with other meteorological and crop data as input parameters to a summary model of vegetation response on a regional basis.

6.2 DRY AND WETFALL ACIDIC OR ACIDIFYING POLLUTANTS

Some scientists feel that dry (acid aerosols) and wetfall acidic pollutants (acidic rain) are only important as more than additive, response inducing agents with other air pollutants. Clear evidence for causation of direct effects of exposure to increased hydrogen ion concentration on crop and tree surfaces in actual, natural terrestrial field environments is lacking. There are two mechanistic process models (Andersson et al. 1980; Haines and Waide 1980) and one statistical model (Medeiros et al. 1983) for acidic precipitation, but these are not sufficiently developed to lead us to recommend their use in other projects. Until, and unless, evidence for field effects on vegetation is established by observations using physiological ecology and pathology, truthful, reliable, and useful vegetation response models cannot be assembled. Unfortunately, standard precipitation meteorology observations do not include leaf wetness measurements as influenced by dew condensation or fog interception. These processes of surface wetting followed by exposure to dryfall appear to be a significant mechanism in inducing vegetation effects.

6.2.1 Local, Point-Source Oriented Applications

For the assessment of pollutant effects on crop and tree species in local areas around point sources of sulphur, oxides of nitrogen, and pollutant mixtures, comprehensive mechanistic process models of vegetation growth could be used. In these studies, only a few to several field study sites would be needed for application, in contrast to regional scale applications.

6.2.2 Sulphur Dioxide or Hydrogen Sulphide

For gaseous sulphur pollutants and responses of small grain crops, we recommend that Coughenour's (1981) model (Table 8B) be adapted to the needs of an assessment program. Such an approach should include enhancements to the pollutant exposure interaction, to account for the discontinuous, fluctuating air quality regimes of varying durations and peaks.

In forest environments with SO_2 exposures, we recommend the adaptation of the Kercher and Axelrod (1981) SILVA model. This needs to be retrofitted, however, with more realistic air pollutant exposure kinetics such as those in the Nosal (1983, 1984) models.

6.2.3 Oxides of Nitrogen and Pollutant Mixtures

Unfortunately, we cannot recommend any biological process models of field effects caused by oxides of nitrogen or pollutant mixtures for crop or tree species because we have not found any. The statistical models for nitrogen dioxide (Heck and Tingey 1979) and for pollutant mixtures (Medeiros et al. 1983; Rowe and Chestnut 1985) are the only ones in this category of which we are aware.

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8. APPENDICES

The appendices contain the mathematical equations for some of the models referenced in Tables 7A, B and 8A, B.

Equations for empirical statistical models shown in Table 7:

Benson et al. (1982)
Heagle et al. (1986)
Heck and Tingey (1979)
Heck et al. (1982)
Heck et al. (1984b)
Larsen and Heck (1976)
Loehman and Wilkinson (1983)
Medeiros et al. (1983)
Nosal (1983)
Nosal (1984)
Oshima et al. (1976)
Rowe and Chestnut (1985)
Stevens and Hazelton (1976)

Equations for mechanistic process models shown in Table 8:

Coughenour (1981)
Kercher (1980)
Kercher and Axelrod (1981)
King et al. (1983)
Mortensen (1984)

Computer program equations for the SUCROS Summary Model of small grains (non-pollution):

van Keulen et al. (1982)

Those models for which we could not find published mathematical equations, or statistical regression equations for which coefficients were not published, are not included in the appendices.

For specific literature citations included within any given model, the reader is referred to the original publication of the model itself, as cited in this report.

8.1 EQUATIONS FOR EMPIRICAL STATISTICAL MODELS

Benson, F.J., S.V. Krupa, P.S. Teng, and D.E. Welsch. 1982. Economic assessment of air pollution damage to agricultural and silvicultural crops in Minnesota. Final Report to Minnesota Pollution Control Agency, Roseville, Minnesota. 270 pp.

In general, the effect of any stress factor at one point in a crop's growth may be expressed in terms of a proportion of response relative to a check. This check may be the crop's response under conditions of zero stress or, in the case of ozone and sulphur dioxide, conditions with background ambient concentrations. The general empirical model is expressed as:

$$Y = f(X_{t_i}) \ . \ . \ . \qquad [1]$$

where

Y = proportion of reduction in response parameter, e.g., dry matter or yield, and
X_i = stress dosage parameter at time t_i.

With linear least squares approximation, an example of a functional relationship may be:

$$Y = b_0 + b_1X + b_2X^2 \ . \ . \ . \qquad [2]$$

where

Y = proportion of yield loss, and
X = dose at a crop development stage.

To develop a method for estimating crop response over a growing season, it is essential that the dynamic "episodal" nature of pollutant concentrations be accounted for. The approach adopted is a dynamic matrix model, where for each specified time interval, dt, a functional relationship was developed, as in equation [2]. A proportion of yield reduction, Δy, is incurred during each time interval. The net crop response over a growing season is:

$$\int_1^n y \cdot dt$$

where

n = maximum number of growing days.

The time step for integration, dt, was dependent on the specific crop and the raw data used in the model development. For example, with alfalfa, where pollutants have a direct effect on the economic biomass, dt = 1 day. With a cereal, where pollutants have an indirect loss effect, i.e., the plant part affected by pollution is different from the part with economic value (the grain), dt was a larger time step.

continued...

Three summary statistics were tested for characterizing pollutant dosage on a daily basis. These were:

$$\frac{\sum_{i=1}^{n} h_i}{n}$$ the mean dose per hour when dose exceeds ambient background.

$$\frac{\sum_{i=1}^{n} h_i}{24}$$ the mean dose per hour over a standardized 24 hour period.

$$\sum_{i=1}^{n} h_i$$ the total dose per day.

Depending on the size of the time interval, these daily statistics were combined over the appropriate number of days.

Heagle, A.S., V.M. Lesser, J.O. Rawlings, W.W. Heck, and R.B. Philbeck. 1986. Responses of soybeans to chronic doses of ozone applied as constant or proportional additions to ambient air. Phytopathology 76:51-56.

Equations for the regression of seed yield of cultivar Davis soybeans on chronic doses of O_3 added in constant or proportional amounts to the O_3 in ambient air.

Polynomial models:[a]

Constant addition:[b]

$$y = \underset{(16)}{549} - \underset{(226)}{2723x}$$

Proportional addition:

$$y = \underset{(28)}{426} + \underset{(1174)}{3637x} - \underset{(10,482)}{59,814x^2}$$

Ignoring method of addition (reduced model):

$$y = \underset{(64)}{357} + \underset{(3987)}{9514x} - \underset{(68,869)}{200,060x^2} + \underset{(352,771)}{945,529x^3}$$

Full (segmented) polynomial models:[c]

$$y = \underset{(33)}{469} - \underset{(891)}{44x} \text{ (for } x \leq 0.044 \text{ ppm)}$$

$$y = \underset{(33)}{469} - \underset{(362)}{3630}(x - 0.044) \text{ (for } x > 0.044 \text{ and constant addition)}$$

$$y = \underset{(33)}{469} - \underset{(467)}{4112}(x - 0.044) \text{ (for } x > 0.044 \text{ and proportional addition)}$$

Weibull models:[d]

Constant addition:

$$y = 490\, e^{-(x/0.126)^{2.17}}$$
(20, 0.007, 0.44)

Proportional addition:

$$y = 479\, e^{-(x/0.103)^{3.89}}$$
(12, 0.003, 0.67)

Ignoring method of addition:

$$y = 492\, e^{-(x/0.121)^{2.26}}$$
(21, 0.006, 0.43)

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continued...

a y = yield (g) of seeds per metre of row; x = O_3 dose characterized as the seasonal 7 h/day mean concentration (ppm). Standard errors for each parameter estimate are shown in parentheses.

b The quadratic equation (with standard errors in parentheses) for constant additions was:

$$y = 500\ (31) - 694x\ (1063) - 15{,}901x^2\ (8145).$$

c The segmented polynomial model provides for a linear response (b_1 = -43.8x) to O_3 levels $\leq$ 0.044 ppm and a different linear response above 0.044 ppm for constant addition, b_c = -3650, and for proportional addition, b_p = -4112, and x = O_3 concentration.

d For the Weibull model ($y = \alpha\ e^{[-x/\sigma]^c}$); y = estimated yield of seeds (g) per metre of row; x = O_3 dose as seasonal 7 h/day mean concentration (ppm); α = maximum seed yield at 0 ppm O_3; σ = O_3 concentration at which α is reduced by 63%; and c is a dimensionless shape parameter. Standard errors in parentheses are for α, σ, and c, respectively.

Heck, W.W. and D.T. Tingey. 1979. Nitrogen dioxide: time-concentration model to predict acute foliar injury. U.S. Environmental Protection Agency, EPA-600/3-79-057. Corvallis, Oregon. 16 pp.

Time-concentration response equations for a selected group of plants exposed to nitrogen dioxide.[a]

Plants by Name (Common, Cultivars)	Equation ($C = A_0 + A_1\ I + A_2/T$)[b]	R^2[c]	Concentrations (ppm) to produce the I (in %) in T (h): I=5, T=1	I=5, T=8	I=50, T=1	I=50, T=8
Susceptible						
Oats (Clintland 64)	C=1.45+0.13 I+2.39/T	0.76	4.5	2.3	10.3	8.3
Radish (Cherry Belle)	C=2.43+0.14 I+1.02/T	0.83	4.1	3.2	10.5	9.6
Oats (329-80)	C=1.75+0.15 I+3.24/T	0.56	5.7	2.9	12.5	9.7
Bromegrass (Sac Smooth)	C=2.49+0.16 I+1.90/T	0.71	5.2	3.5	12.4	10.7
Begonia (Thousand Wonders White)	C=2.45+0.15 I+2.99/T	0.63	6.2	3.5	12.9	10.3
Chrysanthemum (Oregon)	C=3.16+0.16 I+2.14/T	0.72	6.1	3.7	13.3	11.4
Oats (Pendek)	C=2.79+0.14 I+2.88/T	0.50	6.4	3.8	12.7	10.2
Wheat (Wells)	C=2.80+0.13 I+2.94/T	0.52	6.4	3.8	10.2	7.7
Sultana (White Imp)	C=3.93+0.13 I+1.73/T	0.67	6.3	4.8	12.2	10.7
Broccoli (Calabreese)	C=3.07+0.20 I+2.94/T	0.53	7.0	4.5	16.0	13.4
Periwinkle (Bright Eyes)	C=2.92+0.23 I+3.02/T	0.55	7.1	4.5	17.4	14.8
Intermediate						
Cotton (Paymaster)	C=2.97+0.23 I+1.94/T	0.58	7.1	5.3	17.4	15.7
Cotton (Acala 4-42)	C=3.68+0.22 I+3.15/T	0.50	7.9	5.2	17.8	15.1
Tobacco (Bel B)	C=3.62+0.21 I+3.98/T	0.38	8.7	5.2	18.1	14.6
Tobacco (Bel W3)	C=3.65+0.18 I+4.40/T	0.31	9.0	5.2	17.1	13.2
Tobacco (White Gold)	C=4.03+0.30 I+3.56/T	0.40	9.1	6.0	22.6	19.5
Tolerant						
Tobacco (Burley 21)	None	1 of 36 plants injured; 0.5 h, 26 ppm, 33 percent.				
Corn (Pioneer 509-W)	None	4 of 36 plants injured; all injuries were 1.6 percent.				
Corn (Golden Cross)	None	1 of 36 plants injured; 7.0 h, 6 ppm, 7 percent.				
Azalea (Alaska)	None	1 of 36 plants injured; 1.0 h, 17 ppm, 5 percent.				
Sorghum (Martin)	None	0 of 36 plants injured.				
Cucumber (Long Marketer)	None	0 of 36 plants injured.				

continued...

[a] Equations were developed from exposures limited in time (0.5 - 7.0 h) and denote acute injury symptoms to the plants. Concentrations used ranged from 1 to 20 ppm of nitrogen dioxide. Plants are grouped in three susceptibility categories.

[b] C is nitrogen dioxide concentration in ppm; I is percent injury; T is time in h; and A_0, A_1, and A_2 are constants (partial regression coefficients) specific for pollutant, plant species, and environmental conditions used.

[c] R^2, multiple correlation coefficient squared which represents the percent variation explained by the model.

Heck, W.W., O.C. Taylor, R. Adams, G. Bingham, J. Miller, E. Preston, and L. Weinstein. 1982. Assessment of crop loss from ozone. Journal of the Air Pollution Control Association 32(4): 353-361.

Linear regression models of crop yield as a function of O_3 concentration.

Crop		Linear Functions[a] ($\pm$SE)[b]		R^2	Predicted Yield[c] in g/plant ($\pm$SE) 0.025 ppm	0.06 ppm	0.10 ppm
Corn	y =	247.8 -	260 x	0.65	241.3	232.2	221.8
(Coker 16)		($\pm$6.3)	($\pm$68)		($\pm$5.2)	($\pm$3.2)	($\pm$3.4)
Soybean	y =	23.5 -	126 x	0.96	20.3	15.9	10.9
(Corsoy)		($\pm$0.7)	($\pm$10)		($\pm$0.5)	($\pm$0.3)	($\pm$0.5)
Soybean - 1977	y =	96.6 -	385 x	0.90	87.0	73.5	58.1
(Davis)		($\pm$7.5)	($\pm$78)		($\pm$5.9)	($\pm$4.0)	($\pm$3.6)
Soybean - 1978	y =	95.3 -	309 x	0.99	87.6	73.8	64.4
(Davis)		($\pm$9.3)	($\pm$109)		($\pm$6.9)	($\pm$4.4)	($\pm$4.7)
Kidney Bean	y =	16.8 -	31 x	0.84	16.1	14.9	13.7
(Calif. Light Red)		($\pm$0.6)	($\pm$7)		($\pm$0.5)	($\pm$0.4)	($\pm$0.3)
Lettuce, Head	y =	1065.7 -	5978 x	0.94	916.2	707.0	467.9
(Empire)		($\pm$66.4)	($\pm$701)		($\pm$50.3)	($\pm$30.5)	($\pm$24.2)
Peanut[d]	y =	173.2 -	1046 x	0.99	147.1	110.4	68.6
(NC-6)		($\pm$3.6)	($\pm$42)		($\pm$2.6)	($\pm$1.6)	($\pm$1.8)
Spinach	y =	22.7 -	106 x	0.98	20.1	16.3	12.1
(America)		($\pm$2.1)	($\pm$23)		($\pm$1.6)	($\pm$1.1)	($\pm$1.1)
Spinach	y =	42.1 -	193 x	0.93	37.3	30.5	22.8
(Hybrid 7)		($\pm$4.9)	($\pm$53)		($\pm$3.8)	($\pm$2.6)	($\pm$2.6)
Spinach	y =	46.1 -	238 x	0.94	40.1	31.8	22.3
(Viroflay)		($\pm$4.5)	($\pm$27)		($\pm$3.5)	($\pm$2.4)	($\pm$2.4)
Spinach	y =	23.3 -	121 x	0.996	20.2	16.0	11.2
(Winter Bloomsdale)		($\pm$8.5)	($\pm$49)		($\pm$1.9)	($\pm$1.3)	($\pm$1.3)
Turnip[d]	y =	12.9 -	94 x	0.86	10.6	7.3	3.5
(Just Right)		($\pm$0.5)	($\pm$8)		($\pm$0.4)	($\pm$0.2)	($\pm$0.4)
Turnip[d] (Purple	y =	7.2 -	49 x	0.94	6.0	4.3	2.3
Top White Globe)		($\pm$0.3)	($\pm$5)		($\pm$0.2)	($\pm$0.2)	($\pm$0.3)
Turnip	y =	5.3 -	36 x	0.89	4.4	3.1	1.7
(Shogoin)		($\pm$0.3)	($\pm$4)		($\pm$0.2)	($\pm$0.1)	($\pm$0.2)
Turnip[d]	y =	18.1 -	116 x	0.75	15.2	11.1	6.5
(Tokyo Cross)		($\pm$1.5)	($\pm$24)		($\pm$1.1)	($\pm$0.8)	($\pm$1.3)
Wheat	y =	6.6 -	18 x	0.92	6.2	5.5	4.8
(Blueboy II)		($\pm$0.3)	($\pm$3)		($\pm$0.2)	($\pm$0.1)	($\pm$0.1)
Wheat	y =	5.8 -	21 x	0.98	5.3	4.5	3.7
(Coker 47-27)		($\pm$0.1)	($\pm$2)		($\pm$0.2)	($\pm$0.1)	($\pm$0.1)
Wheat[d]	y =	5.7 -	16 x	0.82	5.3	4.7	4.1
(Holly)		($\pm$0.3)	($\pm$3)		($\pm$0.2)	($\pm$0.1)	($\pm$0.1)
Wheat	y =	4.9 -	12 x	0.88	4.6	4.2	3.7
(Oasis)		($\pm$0.2)	($\pm$2)		($\pm$0.2)	($\pm$0.1)	($\pm$0.1)

continued...

[a] Linear regression model of the form $y = b_0 + b_1 x$, where y = yield in g/plant and x = seasonal 7-h/day mean O_3 concentration.

[b] The standard error term was calculated using the mean square error from the analysis of variance.

[c] Values may differ slightly from those predicted by the equations due to a rounding of numbers in the functions shown. The 0.06 ppm seasonal 7-h/day mean O_3 concentration is the maximum mean concentration expected in many parts of the US when the one-hour standard of 0.12 ppm is just met. The 0.10 ppm seasonal value was arbitrarily used as a maximum concentration to consider and approximates the NF-3 treatment.

[d] More complex models account for significantly more of the variation than these simple linear models.

Plateau-linear models of crop yield as a function of O_3 concentration.[a]

Plateau-Linear Functions[b]	R^2	Predicted Yield[c] (g/plant) 0.025 ppm ($\pm$SE)	0.06 ppm ($\pm$SE)	0.10 ppm ($\pm$SE)	Predicted % Yield Reduction at x = 0.06 ppm ($\pm$SE)
Peanut (NC-6)					
$y=142.3$ if $x\leq\theta=0.037$	0.99	142.3	115.0	68.6	19.2
$y=184.6-1160x$ if $x>0.037$		($\pm$3.3)	($\pm$3.6)	($\pm$5.2)	($\pm$1.1)
Turnip (Just Right)					
$y=10.7$ if $x\leq\theta=0.038$	0.96	10.7	7.8	2.8	26.6
$y=15.5-127x$ if $x>0.038$		($\pm$0.4)	($\pm$0.6)	($\pm$1.2)	($\pm$4.1)
Turnip (Purple Top White Globe)					
$y=6.0$ if $x\leq\theta=0.034$	0.99	6.0	4.4	2.0	26.0
$y=8.1-60x$ if $x>0.034$		($\pm$0.3)	($\pm$0.4)	($\pm$0.6)	($\pm$3.4)
Turnip (Tokyo Cross)					
$y=14.8$ if $x\leq\theta=0.054$	0.94	14.8	12.7	4.4	13.9
$y=27.0-226x$ if $x>0.054$		($\pm$1.2)	($\pm$1.2)	($\pm$2.9)	($\pm$3.8)
Wheat (Holly)					
$y=4.9$ if $x\leq\theta=0.087$	0.99	4.9	4.9	4.4	0
$y=8.2-38x$ if $x>0.087$		($\pm$0.1)	($\pm$0.1)	($\pm$0.2)	(-)

a This includes only those data sets for which the fit was significantly improved over the linear model. The O_3 is expressed as the seasonal 7-h/day mean concentration.

b $y=b_0$ if $x\leq\theta$; $y=(b_0-b_1\theta)+b_1x$ if $x>\theta$. The θ is the threshold concentration (ppm) below which yield (y) is unchanged at a value b_0; b_1 is the slope of the linear portion if the O_3 concentration (x) is greater than θ.

c Values may differ slightly from those predicted by the equations due to a rounding of numbers in the functions shown. The 0.06 ppm seasonal 7-h/day mean O_3 concentration is the maximum mean concentration expected in many parts of the US when the one-hour standard of 0.12 ppm is just met, while 0.10 ppm was arbitrarily used as a maximum 7-h/day concentration for comparison.

Percent yield reduction as a function of O_3 concentration.[a]

Crop	Linear Function[b]	Predicted % Yield Reduction at Two O_3 Concentrations.[d] ($\pm$SE) 0.06 ppm	0.10 ppm
Corn (Coker 16)	Y = -2.7 + 108 x	3.83 $\pm$ 1.0	8.1 $\pm$ 2.1
Soybean (Corsoy)	Y = -15.5 + 621 x	21.7 $\pm$ 1.4	46.5 $\pm$ 2.9
Soybean - 1977 (Davis)	Y = -11.1 + 443 x	15.5 $\pm$ 2.4	33.2 $\pm$ 5.1
Soybean - 1978 (Davis)	Y = -8.8 + 353 x	12.3 $\pm$ 3.6	26.4 $\pm$ 7.7
Kidney Bean (Calif. Light Red)	Y = -4.8 + 193 x	6.8 $\pm$ 1.3	14.5 $\pm$ 2.8
Lettuce, Head (Empire)	Y = -16.3 + 652 x	22.8 $\pm$ 1.7	48.9 $\pm$ 3.6
Peanut (NC-6)	Y = -17.8 $\pm$ 711 x[c]	24.9 $\pm$ 0.7	53.3 $\pm$ 1.5
Spinach (America)	Y = -13.2 + 527 x	18.5 $\pm$ 3.0	39.6 $\pm$ 6.4
Spinach (Hybrid 7)	Y = -13.0 + 517 x	18.1 $\pm$ 3.7	38.9 $\pm$ 8.0
Spinach (Viroflay)	Y = -14.8 + 594 x	20.7 $\pm$ 3.1	44.4 $\pm$ 6.6
Spinach (Winter Bloomsdale)	Y = -14.9 + 599 x	20.9 $\pm$ 3.4	44.8 $\pm$ 7.3
Turnip (Just Right)	Y = -22.1 + 887 x[c]	31.0 $\pm$ 2.1	66.4 $\pm$ 4.5
Turnip (Purple Top White Globe)	Y = -20.5 + 817 x[c]	28.6 $\pm$ 2.4	61.4 $\pm$ 5.0
Turnip (Shogoin)	Y = -20.5 + 818 x	28.6 $\pm$ 2.6	61.4 $\pm$ 5.5
Turnip (Tokyo Cross)	Y = -19.1 + 763 x[c]	26.8 $\pm$ 4.6	57.4 $\pm$ 9.8
Wheat (Blueboy II)	Y = -7.4 + 290 x	10.4 $\pm$ 1.4	22.3 $\pm$ 3.0
Wheat (Coker 47-27)	Y = -10.1 + 405 x	14.2 $\pm$ 1.2	30.4 $\pm$ 2.6
Wheat (Holly)	Y = -7.5 + 304 x[c]	10.6 $\pm$ 1.5	22.6 $\pm$ 3.3
Wheat (Oasis)	Y = -6.2 + 250 x	8.7 $\pm$ 1.7	18.6 $\pm$ 3.7

a This includes all data sets. The O_3 is expressed as the seasonal 7-h/day mean concentration.

b
$$Y = \frac{100\ b_1}{a}[0.025-x]$$

where Y = predicted percent yield reduction, b_1 = the regression coefficient from the yield model, a = the predicted yield at a seasonal 7-h/day mean O_3 concentration of 0.025 ppm and x = seasonal 7-h/day mean O_3 concentration.

c These models must be considered with caution. More complex models account for significantly more of the variation than these simple linear models. Compare the predicted percent yield reductions for the plateau-linear model at 0.06 ppm to get an idea of the differences.

d Values may differ slightly from those predicted by the equations due to a rounding of numbers in the functions shown. The 0.06 ppm seasonal 7-h/day mean O_3 concentration is the maximum mean concentration expected in many parts of the US when the one-hour standard of 0.12 ppm is just met; the 0.10 ppm was arbitrarily used as a maximum 7-h/day mean O_3 concentration for comparison.

Heck, W.W., W.W. Cure, J.O. Rawlings, L.J. Zaragoza, A.S. Heagle, H.E. Heggestad, R.J. Kohut, L.W. Kress, and P.J. Temple. 1984. Assessing impacts of ozone on agricultural crops: II. Crop yield functions and alternative exposure statistics. Journal of the Air Pollution Control Association 34: 810-817.

Estimates of the parameters and the residual mean squares (RMS) from fitting the Weibull model using four different exposure statistics to describe O_3 concentration.

Estimated Parameters and RMS[a]	Parameter Estimates for Ozone Exposure Statistics[b]			
	M7	P7	M1	P1
<u>Barley</u>				
'Poco'[c], 1982 - Shafter, CA				
$\hat{\alpha}$ (se)	1.988 (0.051)	1.991 (0.049)	1.990 (0.050)	1.989 (0.052)
$\hat{\sigma}$ (se)	0.205 (0.669)	0.322 (0.744)	0.246 (0.651)	0.466 (1.562)
$\hat{c}$ (se)	4.278 (17.15)	4.231 (12.66)	4.385 (15.26)	3.724 (13.51)
RMS (21)	0.0248	0.0245	0.0246	0.0248
<u>Bean, kidney</u>				
'Calif. Light Red'[d], (Full Plots - FP), 1982 - Ithaca, NY				
$\hat{\alpha}$ (se)	2878 (416)	3586 (1444)	3394 (1134)	3776 (2025)
$\hat{\sigma}$ (se)	0.120 (0.013)	0.171 (0.071)	0.130 (0.048)	0.183 (0.100)
$\hat{c}$ (se)	1.171 (0.489)	0.960 (0.641)	0.865 (0.533)	1.000 (0.779)
RMS (7)	30354	30779	31489	28870
'Calif. Light Red'[d], (Partial Plots - PP), 1982 - Ithaca, NY				
$\hat{\alpha}$ (se)	2447 (183)	2437 (122)	2444 (122)	2432 (127)
$\hat{\sigma}$ (se)	0.108 (0.007)	0.187 (0.007)	0.140 (0.006)	0.242 (0.011)
$\hat{c}$ (se)	3.942 (1.733)	4.727 (1.456)	3.88 (1.164)	4.620 (1.839)
RMS (7)	100130	116257	103095	215898
<u>Corn</u>				
'PAG 397', 1981 - Argonne, IL				
$\hat{\alpha}$ (se)	13968 (322)	13928 (311)	13971 (324)	13899 (315)
$\hat{\sigma}$ (se)	0.160 (0.004)	0.244 (0.004)	0.182 (0.005)	0.248 (0.004)
$\hat{c}$ (se)	4.280 (0.723)	6.912 (1.161)	4.349 (0.730)	7.401 (1.293)
RMS (17)	2644143	2391941	2463065	2505320
'Pioneer 3780', 1981 - Argonne, IL				
$\hat{\alpha}$ (se)	12533 (323)	12524 (325)	12552 (329)	12539 (330)
$\hat{\sigma}$ (se)	0.155 (0.004)	0.220 (0.004)	0.176 (0.005)	0.244 (0.004)
$\hat{c}$ (se)	3.091 (0.461)	4.811 (0.734)	3.142 (0.467)	4.987 (0.771)
RMS (17)	774833	697778	773206	740201
<u>Cotton</u>				
'Acala SJ-2', 1981 - Shafter, CA, (Irrigated-I)				
$\hat{\alpha}$ (se)	5546 (356)	5699 (489)	5526 (379)	5746 (506)
$\hat{\sigma}$ (se)	0.199 (0.020)	0.253 (0.026)	0.211 (0.020)	0.268 (0.027)
$\hat{c}$ (se)	1.228 (0.402)	1.182 (0.415)	1.315 (0.419)	1.214 (0.423)
RMS (9)	80907	117382	85315	113000
'Acala SJ-2', 1981 - Shafter, CA, (Droughted - D)				
$\hat{\alpha}$ (se)	3323 (278)	3323 (292)	3317 (272)	3323 (387)
$\hat{\sigma}$ (se)	0.269 (0.076)	0.351 (0.101)	0.280 (0.073)	0.366 (0.128)
$\hat{c}$ (se)	1.969 (1.308)	1.980 (1.286)	2.131 (1.389)	2.027 (1.706)
RMS (9)	232623	267524	237305	261563

continued...

Estimated Parameters and RMS[a]	Parameter Estimates for Ozone Exposure Statistics[b]			
	M7	P7	M1	P1
'Acala SJ-2'[e], 1982 - Shafter, CA, (Irrigated - I)				
$\hat{\alpha}$ (se)	5872 (555)	6192 (990)	5901 (580)	6321 (1038)
$\hat{\sigma}$ (se)	0.088 (0.007)	0.174 (0.023)	0.108 (0.009)	0.211 (0.032)
$\hat{c}$ (se)	2.100 (0.796)	1.374 (0.700)	2.084 (0.798)	1.197 (0.587)
RMS (9)	417881	436672	427681	524417
'Acala SJ-2'[e], 1982 - Shafter, CA, (Droughted - D)				
$\hat{\alpha}$ (se)	4938 (412)	4934 (403)	4947 (417)	4926 (404)
$\hat{\sigma}$ (se)	0.094 (0.008)	0.187 (0.018)	0.115 (.009)	0.213 (0.020)
$\hat{c}$ (se)	3.333 (1.537)	2.860 (1.504)	3.355 (1.551)	2.997 (1.572)
RMS (9)	443277	395639	441216	404471
'Stoneville 213'[f], 1982 - Raleigh, NC				
$\hat{\alpha}$ (se)	3686 (140)	3982 (252)	3732 (154)	3828 (220)
$\hat{\sigma}$ (se)	0.112 (0.004)	0.161 (0.006)	0.127 (0.004)	0.175 (0.005)
$\hat{c}$ (se)	2.577 (0.416)	2.005 (0.382)	2.638 (0.440)	3.061 (0.580)
RMS (21)	52171	63823	50211	93827
<u>Peanut</u>				
'NC-6', 1980 - Raleigh, NC				
$\hat{\alpha}$ (se)	7485 (231)	7705 (299)	7586 (258)	8381 (501)
$\hat{\sigma}$ (se)	0.111 (0.002)	0.167 (0.004)	0.128 (0.003)	0.186 (0.006)
$\hat{c}$ (se)	2.249 (0.225)	2.272 (0.254)	2.180 (0.228)	2.025 (0.264)
RMS (17)	109603	168540	122330	251656
<u>Sorghum</u>				
'DeKalb-28', 1982 - Argonne, IL				
$\hat{\alpha}$ (se)	8137 (218)	8122 (201)	8156 (235)	8138 (211)
$\hat{\sigma}$ (se)	0.296 (0.135)	0.305 (0.075)	0.361 (0.171)	0.349 (0.093)
$\hat{c}$ (se)	2.217 (1.229)	3.984 (2.098)	2.161 (1.228)	3.924 (2.174)
RMS (17)	195875	197090	197626	205486
<u>Soybean</u>				
'Corsoy', 1980 - Argonne, IL				
$\hat{\alpha}$ (se)	2785 (179.3)	2817 (201)	2808 (198)	2799 (196)
$\hat{\sigma}$ (se)	0.133 (0.010)	0.197 (0.013)	0.167 (0.012)	0.242 (0.013)
$\hat{c}$ (se)	1.952 (0.587)	2.122 (0.663)	1.917 (0.595)	2.572 (0.798)
RMS (7)	32514	37589	33667	28457
'Davis'[f], 1981 - Raleigh, NC				
$\hat{\alpha}$ (se)	5593 (863)	5729 (1124)	6094 (1366)	6620 (3626)
$\hat{\sigma}$ (se)	0.128 (0.019)	0.205 (0.035)	0.139 (0.038)	0.201 (0.111)
$\hat{c}$ (se)	0.872 (0.284)	1.000 (0.378)	0.778 (0.305)	1.000 (0.736)
RMS (43)	91452	141738	97635	236429
'Davis'[g,h], 1982 - Raleigh, NC, (Constant add. - CA)				
$\hat{\alpha}$ (se)	4931 (227)	5308 (544)	4968 (250)	5473 (737)
$\hat{\sigma}$ (se)	0.128 (0.008)	0.248 (0.023)	0.151 (0.009)	0.231 (0.015)
$\hat{c}$ (se)	2.144 (0.500)	1.369 (0.501)	2.129 (0.578)	1.628 (0.711)
RMS (7)	141799	415352	150747	247265
'Davis'[g], 1982 - Raleigh, NC, (Proport. add. - PA)				
$\hat{\alpha}$ (se)	4805 (106)	4917 (146)	4810 (108)	5037 (232)
$\hat{\sigma}$ (se)	0.103 (0.003)	0.233 (0.009)	0.137 (0.004)	0.267 (0.011)
$\hat{c}$ (se)	4.077 (0.648)	2.554 (0.412)	3.763 (0.619)	2.540 (0.601)
RMS (7)	124407	113383	128122	144331

continued...

Estimated Parameters and RMS[a]	Parameter Estimates for Ozone Exposure Statistics[b]			
	M7	P7	M1	P1
'Essex'[f], 1981 - Beltsville, MD				
$\hat{\alpha}$ (se)	4562 (608)	4487 (544)	4622 (600)	4538 (565)
$\hat{\sigma}$ (se)	0.187 (0.124)	0.194 (0.063)	0.168 (0.077)	0.207 (0.057)
$\hat{c}$ (se)	1.543 (1.505)	2.676 (2.128)	2.025 (1.69)	2.997 (2.184)
RMS (25)	232455	232643	226924	227660
'Williams'[f], 1981 - Beltsville, MD				
$\hat{\alpha}$ (se)	4992 (659)	4954 (592)	4969 (569)	5037 (619)
$\hat{\sigma}$ (se)	0.211 (0.120)	0.214 (0.067)	0.174 (0.067)	0.228 (0.065)
$\hat{c}$ (se)	1.100 (0.901)	1.740 (1.206)	1.729 (1.171)	1.936 (1.290)
RMS (25)	127464	124577	138543	114483
'Forrest'[f,i,j], 1982 - Beltsville, MD, (Irrigated - I)				
$\hat{\alpha}$ (se)	4333 (366)	4391 (371)	4369 (388)	4316 (356)
$\hat{\sigma}$ (se)	0.171 (0.041)	0.224 (0.041)	0.190 (0.044)	0.244 (0.041)
$\hat{c}$ (se)	2.752 (1.872)	3.455 (2.244)	2.967 (2.067)	4.709 (3.518)
RMS (11)	374947	363968	401359	422091
'Forrest'[f,i,j], 1982 - Beltsville, MD, (Droughted - D)				
$\hat{\alpha}$ (se)	5384 (706)	5669 (905)	5661 (944)	5893 (1205)
$\hat{\sigma}$ (se)	0.205 (0.041)	0.271 (0.045)	0.216 (0.035)	0.312 (0.046)
$\hat{c}$ (se)	1.000 (0.538)	1.000 (0.577)	1.000 (0.586)	1.000 (0.648)
RMS (11)	204273	177953	177994	181555
'Williams'[f,i,j], 1982 - Beltsville, MD, (Irrigated - I)				
$\hat{\alpha}$ (se)	5884 (389)	5826 (326)	5913 (383)	5769 (302)
$\hat{\sigma}$ (se)	0.162 (0.017)	0.213 (0.017)	0.176 (0.016)	0.233 (0.015)
$\hat{c}$ (se)	1.577 (0.504)	2.226 (0.649)	1.865 (0.565)	2.893 (0.803)
RMS (11)	124318	132923	145116	131361
'Williams'[f,i,j], 1982 - Beltsville, MD, (Droughted - D)				
$\hat{\alpha}$ (se)	4480 (739)	5126 (942)	5114 (985)	5339 (1259)
$\hat{\sigma}$ (se)	0.217 (0.059)	0.287 (0.064)	0.229 (0.050)	0.328 (0.061)
$\hat{c}$ (se)	1.000 (0.654)	1.000 (0.702)	1.000 (0.715)	1.000 (0.781)
RMS (11)	189004	169920	171588	159911
'Hodgson'[d], 1981 - Ithaca, NY, (Full plots - FP)				
$\hat{\alpha}$ (se)	2590 (439)	2851 (1025)	2685 (875)	3059 (1817)
$\hat{\sigma}$ (se)	0.138 (0.026)	0.188 (0.042)	0.174 (0.030)	0.225 (0.100)
$\hat{c}$ (se)	1.000 (0.609)	1.000 (0.865)	1.000 (0.903)	1.000 (1.180)
RMS (7)	41226	49037	49268	74253
<u>Tomato</u>				
'Murrieta'[f,j,k], 1981 - Tracy, CA				
$\hat{\alpha}$ (se)	32.9 (1.10)	33.2 (1.58)	-	33.1 (1.36)
$\hat{\sigma}$ (se)	0.142 (0.026)	0.209 (0.048)	-	0.241 (0.044)
$\hat{c}$ (se)	3.807 (1.938)	2.832 (1.500)	-	3.447 (1.594)
RMS (28)	11.95	13.16	-	13.75
'Murrieta'[e,f,j], 1982 - Tracy, CA				
$\hat{\alpha}$ (se)	32.3 (1.385)	35.5 (11.44)	32.7 (1.656)	36.8 (16.20)
$\hat{\sigma}$ (se)	0.082 (0.025)	0.589 (0.626)	0.145 (0.052)	0.690 (0.787)
$\hat{c}$ (se)	3.050 (1.871)	1.000 (1.733)	2.668 (1.825)	0.977 (2.063)
RMS (28)	10.28	10.36	10.36	11.01

continued...

Estimated Parameters and RMS[a]	Parameter Estimates for Ozone Exposure Statistics[b]			
	M7	P7	M1	P1
Wheat, winter				
'Abe'[1], 1982 - Argonne, IL				
$\hat{\alpha}$ (se)	5363 (246)	5381 (242)	5392 (267)	5508 (295)
$\hat{\sigma}$ (se)	0.143 (0.010)	0.202 (0.010)	0.174 (0.012)	0.228 (0.010)
$\hat{c}$ (se)	2.423 (0.666)	3.148 (0.824)	2.351 (0.671)	3.285 (0.834)
RMS (17)	161418	165453	165621	190052
'Arthur 71', 1982 - Argonne, IL				
$\hat{\alpha}$ (se)	4684 (156)	4715 (154)	4709 (169)	4837 (190)
$\hat{\sigma}$ (se)	0.148 (0.007)	0.209 (0.008)	0.180 (0.009)	0.234 (0.008)
$\hat{c}$ (se)	2.154 (0.411)	2.711 (0.491)	2.119 (0.418)	2.886 (0.510)
RMS (17)	64939	76907	63462	94348
'Roland'[1], 1982 - Argonne, IL				
$\hat{\alpha}$ (se)	5479 (312)	5331 (229)	5598 (373)	5517 (279)
$\hat{\sigma}$ (se)	0.113 (0.005)	0.171 (0.005)	0.136 (0.006)	0.194 (0.005)
$\hat{c}$ (se)	1.633 (0.288)	2.368 (0.349)	1.572 (0.296)	2.669 (0.397)
RMS (17)	91726	97698	91113	160598
'Vona', 1982 - Ithaca, NY				
$\hat{\alpha}$ (se)	7857 (2111)	8750 (3286)	11133 (6890)	13998 (12737)
$\hat{\sigma}$ (se)	0.053 (0.016)	0.082 (0.034)	0.052 (0.033)	0.072 (0.064)
$\hat{c}$ (se)	1.000 (0.341)	1.000 (0.409)	1.000 (0.487)	1.000 (0.619)
RMS (17)	294084	453900	351597	430977

[a] The estimated parameters ($\hat{\alpha}$, $\hat{\sigma}$, $\hat{c}$) are given with standard errors in parentheses; the residual mean square (RMS) has the degrees of freedom in parentheses.

[b] All $\hat{\sigma}$ estimates are in ppm. With the following exceptions, all estimates of $\hat{\alpha}$ are in units of seed yield (kg/ha): barley--seed weight (g per head); tomato (both years)--fresh weight (kg per plot); cotton--lint + seed weight (kg/ha); peanut--pod weight (kg/ha). In cases where the estimated $\hat{c}$ parameter is exactly 1.0, it has been bounded from below to obtain convergence in the nonlinear model fitting routine. The parameters were estimated from data not showing the expected Weibull form. Caution should be used in interpreting these Weibull models. Other models might better describe the behaviour observed in these experiments. The $\hat{\sigma}$ and $\hat{c}$ estimates may be slightly different than values in Heck et al. because individual plot data were used to calculate the O_3 statistics.

[c] The exposures started late in this experiment so the estimate of loss related to O_3 concentration may be conservative.

[d] "Full" plots are chambers in which the plants were left undisturbed for the entire growing season and "partial" plots are those from which some plants were periodically removed to obtain physiological data.

[e] Weather during the 1982 growing season in California was radically different from that in 1981; rainfall was higher and temperatures were lower in 1982.

continued...

[f] Sulphur dioxide was part of these experimental designs. A bivariate Weibull model was fit to the 1981 Davis, the 1981 Essex, and the Williams soybean data sets while for the other data sets the SO_2 effect was essentially linear and was accounted for by estimation of a separate $\hat{\alpha}$ parameter to accommodate the linear effect.

[g] These two data sets are from the same experiment and utilized the same CF and NF-1 treatment plot yields.

[h] The P1 exposure statistic for the data set would not permit fitting of the Weibull model; therefore, the second highest peak was used.

[i] These four data sets are from a split-plot design with the two cultivars grown in the same treatment plots. The homogeneity test of the proportional response portion of the four models using the M7 statistic indicated that they were homogeneous and a combined proportional response with a single σ and c could be substituted for the four separate models.

[j] These factorial experiments included SO_2 as part of the experimental design and lacked true replication. The error term used in scaling the standard errors and in statistical testing was the residual mean square obtained from the best fitting polynomial model of form: yield = $\beta_0 + \beta_1 O_3 + \beta_2 2SO_2 + \beta_3 O_3{}^2 + \varepsilon$.

[k] The M1 statistic was not available for this data set.

[l] These three data sets are from a split-plot design with the three cultivars grown in the same treatment plots.

Larsen, R. I. and W. W. Heck. 1976. An air quality data analysis system for interrelating effects, standards, and needed source reductions: Part 3. Vegetation injury. Journal of the Air Pollution Control Association 26: 325-333.

In general mathematical terms, the relations can be expressed as

$$z = - \ln m_{ghr} / \ln s_g - p \ln t / \ln s_g + \ln c / \ln s_g$$

where

z is the number of standard deviations that the percent leaf injury is away from the median, ($z = 0$ for 50% injury),

m_{ghr} is the geometric mean concentration of the gas for 1 hour of exposure,

s is the standard geometric deviation for concentrations producing a standard deviation of percent leaf injury,

p is the slope of the percent leaf injury line on logarithmic paper for concentration and duration,

t is the exposure duration in hours, and

c is the pollutant concentration.

Loehman, E. and T. Wilkinson. 1983. Ozone damage to field crops in Indiana. Station Bulletin Number 426, Agricultural Experimental Station, Purdue University, West Lafayette, Indiana. 38 pp.

Regression Equations for Percent Yield Reduction From Ozone

Soybean, cv. Corsoy:
$Z = 619.2\ X - 15.5$

cv. Hodgson:
$Z = 414.7\ X - 10.4$

cv. Davis:
$Z = 349.9\ X - 8.7$

cv. Williams:
$Z = 266.6\ X - 6.6$

cv. Essex:
$Z = 133.4\ X - 3.3$

Z = percent soybean yield reduction,

X = average 7 hour daily maximum ozone concentration above 0.025 ppm.

Field Corn: $Z = 1533.7\ X^2 - 144.6\ X + 26.6$; $X \geq 0.069$ ppm

Winter Wheat: $Z = 2077.8\ X^2 - 73.8\ X + 0.54$

Medeiros, W.H., P.D. Moskowitz, E.A. Coveney, and H.C. Thode, Jr. 1983. Oxidants and acid precipitation: a method for identifying and modeling effects on United States' soybean yield. Paper presented at 76th Annual Meeting, Air Pollution Control Association, Atlanta, Georgia. 1983, June 19-24.

Summary of regression results.[a]

Model[b]	Model Significance	Multiple R^2
1. Univariate		
a. Y = 29.8 -16580.3[H^+]	0.01	0.003
Std. error: 0.24 6665.7		
P: <0.01 0.01		
b. Y = 40.8 -2.1[OXID]	<0.01	0.05
Std. error: 1.17 0.21		
P: <0.01 <0.01		
2. Bivariate		
a. Y = 40.9 -9110.3[H+] -2.0[OXID]	<0.01	0.05
Std. error: 1.17 6553.1 0.21		
P: <0.01 0.17 <0.01		
3. Bivariate with Maturity Zone Indicator		
a. Y = 31.61 +Z_1^9 -0.82[OXID] -2589.60([H^+] [OXID])	<0.01	0.49
Std. error: 1.20 (0.38-0.79) 0.23 1038.72		
P: <0.01 (<0.00-0.51) <0.01 0.01		
b. Y = 32.24 +Z_1^9 -16565.5[H^+] -0.93[OXID]	<0.01	0.49
Std. error: 1.23 (0.38-0.79) 5550.09 0.23		
P: 0.01 (0.01-0.59) <0.01 <0.01		

[a] Y = bushels/acre, H^+ = moles/litre, OXID = 7 hour seasonal average (pphm), and Z19 = zone intercept adjustments.

[b] The number of residual mean square degrees of freedom used in determining the significance of the regression model coefficients is 1871, minus the number of coefficients estimated in the model. The number of degrees of freedom is based on the number of independent residuals, $Y_i - \hat{Y}_i$, where $\hat{Y}_i$ is the model estimate of Y_i. Although the model estimates are also based on estimated data (and are therefore dependent), this does not affect the independencies of the residuals.

Nosal, M. 1983. Atmosphere-biosphere interface: probability analysis and an experimental design for studies of air pollutant-induced plant response. RMD Report 83/25. Research Management Division, Alberta Environment, Edmonton, Alberta. 98 pp.

The following is a synopsis of the numerical regression models obtained after least square fitting. The meaning of the symbols is as follows:

y = specific plant response parameter
x_1 = number of pollutant episodes
x_2 = cumulative integral of the pollutant episodes (concentration and duration)
x_3 = peak pollutant concentration

A. Fumigation Type: Open-Top Chamber Dispensed SO_2 Treatment

1. Plant response: number of pods per plant
   $y = 290 - 18.7x_1 - 0.0043x_2 - 0.013x_3 + 0.354x_1^2$

2. Plant response: seed weight per plant
   $y = 82.6 - 5.80x_1 + 0.0016x_2 + 0.017x_3 + 0.106x_1^2$

3. Plant response: number of seeds per plant
   $y = 626 - 39.3x_1 - 0.012x_2 - 0.0950x_3 + 0.753x_1^2$

4. Plant response: thousand seed weight
   $y = -174 + 13.4x_1 + 0.047x_2 + 0.497x_3 - 0.326x_1^2$

B. Fumigation Type: Open-Top Chamber Dispensed O_3 Treatment

1. Plant response: number of pods per plant
   $y = 0.142 + 1.42x_1 + 0.0002x_2 - 0.273x_3 - 5.64 \sin x_2$

2. Plant response: seed weight per plant
   $y = 28.0 - 0.161x_1 + 0.0001x_2 - 2.05 \sin x_2 - 1.79 \sin x_3$

3. Plant response: number of seeds per plant
   $y = 43.3 + 1.45x_1 + 0.0001x_2 - 0.289x_3 - 10.5 \sin x_2$

4. Plant response: thousand seed weight
   $y = 331 - 1.68x_1 - 0.0001x_2 - 4.16 \sin x_2 - 16.6 \sin x_3$

C. Fumigation Type: Residual-Ambient, Unfiltered, and Filtered Open-Top Chamber Treatment

1. Plant response: pods per plant
   $y = 438 - 8.30x_1 - 0.154x_2 - 0.213x_3 - 0.0154x_6$

2. Plant response: seed weight per plant
   $y = 180 - 3.36x_1 - 0.0863x_2 - 0.0847x_3 - 0.0116x_6$

3. Plant response: number of seeds per plant
   $y = 35.5 - 0.0069x_2 - 0.0421x_3 + 0.0010x_5 - 0.037x_6$

4. Plant response: thousand seed weight
   $y = 1601 - 26.9x_1 - 0.581x_2 - 0.631x_3 - 0.0016x_5$

The meaning of the independent variables is as follows:

x_1 = number of episodes of SO_2
x_2 = integral of the SO_2 concentration
x_3 = peak of the SO_2 concentration
x_4 = number of episodes of O_3
x_5 = integral of the O_3 concentration
x_6 = peak of the O_3 concentration.

Nosal, M. 1984. Atmosphere-biosphere interface: analytical design and a computerized regression model for lodgepole pine response to chronic atmospheric SO_2 exposure. RMD Report 83/26 and 83/27, Research Management Division, Alberta Environment, Edmonton, Alberta. 194 pp.

$$y = \sum_{i=1}^{3} \sum_{n} a_i(n)\, x_i^n + \sum_{i=1}^{3} \sum_{m} \left(b_i^{(m)} \sin \omega_m x_i + c_i^{(m)} \cos \tau_m x_i\right)$$

where

y = annual basal area increment,

x_1 = number of SO_2 episodes,

x_2 = cumulative integral of SO_2 concentrations with respect to time,

x_3 = peak SO_2 concentration, and

$a_i^{(n)}$, $b_i^{(m)}$ = model parameters

Oshima, R.J., M.P. Poe, P.K. Braegelmann, D.W. Balding, and V. Van Way. 1976. Ozone dosage-crop loss function for alfalfa: a standardized method for assessing crop losses from air pollutants. Journal of the Air Pollution Control Association 26(9): 861-865.

Summary of the regression of Moapa 69 alfalfa yield (Y) and leaf to harvest weight ratios (L) with seasonal ozone dosage (D), average daily maximum temperature (TH), average daily minimum temperature (TL), and average daily relative humidity (RH).

$Y = 162.4 - (0.01503 \times D)$				$L = 0.6398 - (1.941 \times 10^{-5} \times D)$			
	df				df		
Matrix	Reg.	Error	r	Matrix	Reg.	Error	r
Y x D	1	7	0.827**	L x D	1	7	0.890**
Y x TH	1	7	0.644	L x TH	1	7	0.373
Y x TL	1	7	0.536	L x TL	1	7	0.089
Y x RH	1	6	0.692	L x RH	1	6	0.610

	df		t-values of regression coefficients				
Matrix	Reg.	Error	D	TH	TL	RH	F
Y x D x TH	2	6	-3.949**	-2.374*			15.449**
Y x D x TL	2	6	-5.364**		3.062*		21.381**
Y x D x RH	2	5	-3.695*			0.085	15.419**
Y x D x TH x TL	3	5	-4.645**	-0.882	1.624		13.987**
Y x D x TH x RH	3	4	-3.129*	-0.720		-0.594	9.463*
Y x D x TL x RH	3	4	-4.162**		1.640	-0.447	14.654*
Y x D x TH x TL x RH	4	3	-3.447*	-0.549	1.375	-0.680	9.148*
L x D x TH	2	6	-4.458**	-0.444			12.032**
L x D x TL	2	6	-4.785**		-0.091		11.573**
L x D x RH	2	5	-3.625*			0.449	11.949*
L x D x TH x TL	3	5	-4.051**	-0.642	-0.497		7.097*
L x D x TH x RH	3	4	-3.371*	0.283		0.550	6.956*
L x D x TL x RH	3	4	-3.500*		-0.159	-0.744	7.441*

* Significant at 0.05 level.
** Significant at 0.01 level.

continued...

Calculated regression equations for significant interactions of Moapa 69 alfalfa yield (Y) and leaf to harvest weight ratios (L) with ozone dosage (D), average daily maximum temperature (TH), average daily minimum temperature (TL) and average daily relative humidity (RH).

Matrix	Equation
Y x D x TH[a]	Y=395.0889-(.0125 x D)-(2.1864 x TH)
Y x D x TL	Y[b]=-166.3028-(.01406 x D)+(5.8919 x TL)
Y x D x RH	Y=168.0667-(.0179 x D)+(.1107 x RH)
Y x D x TH x TL	Y=25.6715-(.0132 x D)-(1.2566 x TH)+(4.3117 x TL)
Y x D x TH x RH	Y=544.3926-(.0167 x D)-(3.457 x TH)-(1.703 x RH)
Y x D x TL x RH	Y=-39.7543-(.0174 x D)+(4.2767 x TL)-(.5351 x RH)
Y x D x TH x TL x RH	Y=237.1657-(.0166 x D)-(2.4218 x TH)+(4.0032 x TL)-(1.7644 x RH)
L x D x TH	$L=.6976-(1.8787\times10^{-5} \times D)-(7.0017\times10^{-4} \times TH)$
L x D x TL	$L=.6549-(1.9455\times10^{-5} \times D)-(2.7253\times10^{-4} \times TL)$
L x D x RH	$L=.6893-(2.3155\times10^{-5} \times D)-(7.730\times10^{-4} \times RH)$
L x D x TH x TL	$L=.8788-(1.8455\times10^{-5} \times D)-(1.4653\times10^{-3} \times TH)-(2.1150\times10^{-3} \times TL)$
L x D x TH x RH	$L=.3014-(2.4361\times10^{-5} \times D)+(1.0964\times10^{-3} \times TH)+(3.5631\times10^{-3} \times RH)$
L x D x TL x RH	$L=.8398-(2.3472\times10^{-5} \times D)-(3.0520\times10^{-4} \times TL)-(3.0976\times10^{-3} \times RH)$

a Temperatures were calculated in degrees Fahrenheit.

b Equations with negative intercepts do not produce negative yields because the minimum temperature values were never lower than 52°F.

Rowe, R. D. and L. G. Chestnut. 1985. Economic assessment of the effects of air pollution on agricultural crops in the San Joaquin Valley (SJV). Journal of the Air Pollution Association 35:728-734.

Crop (Variety)	Equation
I. SJV field data regression results[a]	
Dry beans	$Y = 1.3255 - \underset{(-2.01)}{0.00802}\ (O_3AVE)$, N=87, DF=73, R^2=0.7682
	$Y = 1.1043 - \underset{(-2.24)}{0.000871}\ (O3GE10)$, N=87, DF=73, R^2=0.7710
	$\overline{Y}$ = 1.044 ton/acre $\overline{O_3AVE}$ = 69.2 $\overline{O_3GE10}$ = 69.12
Cotton	$Y = 0.5345 - \underset{(-1.39)}{0.00259}\ (O_3AVE)$, N=72, DF=59, R^2=0.8179
	$Y = 0.4624 - \underset{(-1.73)}{0.000319}\ (O_3GE10)$, N=72, DF=59, R^2=0.8209
	$\overline{Y}$ = 0.440 ton/acre $\overline{O_3AVE}$ = 36.5 $\overline{O_3GE10}$ = 70.1
Grapes	$Y = 7.629 - \underset{(-1.72)}{0.00000166}\ (O_3GE6)^2$, N=72, DF=59, R^2=0.8209
	$\overline{Y}$ = 7.628 tons/acre $\overline{O_3GE6}$ = 494.7
Potatoes	$YP = 1.0872 - \underset{(-1.17)}{0.00185}\ (O_3GE10) - \underset{(-1.30)}{0.0068}(SO_2GE10)$, N=26, DF=15, R^2=0.7613
	$\overline{YP}$ = 1.004 $\overline{O_3GE10}$ = 26.9 $\overline{SO_2GE10}$ = 4.9
II. NCLAN regression results[b]	
Corn (pooled)	$Y = 12277.3 - 301727\ (x^2)$
Wheat (pooled)	$Y = 4852.5 - 169239\ (x^2)$
Grain sorghum (Dekalb, A28+)	$Y = 8157.6 - 72388.3\ (x^2)$
Lettuce (Empire)	$Y = 1065 - 5978\ (x)$
Tomatoes (Murietta)	$Y = 67.1 - 38.85\ (SO_2) - 1703\ (x^2)$
III. Brewer and Aschroft[c]	
Alfalfa	$\%\Delta\ Y = 11.5 - \underset{(-4.6)}{0.00677}\ (O_3GE10) - \underset{(-2.3)}{0.00133}\ (SO_2GE10)$, N=11, DF=8, R^2=0.796, F=10.43

continued...

IV. Legend

Y = yield per acre

YP = yield adjusted by national productivity index

O_3AVE = average hourly O_3 per month summed over growing season in pphm

O_3GE10 = number growing season daytime hours where $O_3 > 10$ pphm

O_3GE6 = number growing season daytime hours where $O_3 > 6$ pphm

SO_2GE10 = number growing season daytime hours where $SO_2 > 10$ pphm

x = average daytime hourly O_3 over the growing season in ppm

SO_2 = average daytime SO_2 over the growing season

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[a] Rowe and Chestnut T-ratios reported in parenthesis under air pollution coefficients. One-tailed statistical tests are appropriate.

[b] Heck et al. (1984)

[c] Rowe and Chestnut regressions on Brewer and Ashcroft results.

Stevens, T. H. and T. W. Hazelton. 1976. Sulfur dioxide pollution and crop damage in the four corners region: a simulation analysis. New Mexico Agricultural Experimental Station Bulletin, 647. Las Cruces, New Mexico.

The effect is described mathematically by:

$$X_s = f(R_s, (C - C_o))$$

$$y_{i,s} = a_{i,s} - b_{i,s}X_s$$

where

R is the species resistance factor for the air pollutant,

C is ambient pollutant concentration producing visible foliar injury,

C_o is the theoretical threshold concentration that can be continually tolerated without foliar injury occurring,

X is percentage leaf area injury,

a is the assumed potential percentage crop yield,

b is a yield-leaf destruction coefficient,

y is the percentage crop yield under polluted air,

i is growth stage, and

s is crop plant species.

This simple model is limited in application because it does not include processes and effects of soil water availability, air temperature, humidity, and solar radiation.

8.2 EQUATIONS FOR MECHANISTIC PROCESS MODELS

Coughenour, M.B. 1981. Relationship of SO_2 dry deposition to a grassland sulfur cycle. Ecological Modelling 13:1-16.

The resistances of diffusion to each of the various sinks are implemented to yield an absolute flux occurring over the solution interval of the simulation (1 day). The relationship

$$F = \frac{C}{r}$$

is used to facilitate this calculation, where F is flux rate (µg SO_2 cm^{-2} s^{-1}), C is concentration (µg SO_2 cm^{-3}) and r is total resistance from the point at which C was measured to the sink (s cm^{-1}). When C is measured at z_r, r_a must be included in r, but when C is measured in the canopy (as is the case here), r_a need not be included in r.

Flux to leaf surfaces or interiors is

$$F = \frac{C}{r} \text{ LAI}$$

where LAI is leaf area index.

Passive deposition onto leaf surfaces is governed by the sink strength of the surface. This sink strength is represented here as a constant leaf surface resistance (r_{su}). The value of r_{su} was found by trial and error to most closely match observed and predicted values of sulphur accumulation on dead leaves. The total resistance for deposition onto live or dead leaf surfaces is then

$$r = r_a + r_b + r_{su}$$

In this model, flux to the soil is found in a similar fashion by use of

$$r = r_a + r_e + r_{sg}$$

where r_a and r_e are the atmospheric resistances to diffusion above and below the canopy, and r_{sg} expresses the surface resistance of the ground.

Over the logarithmic profile of region 1, the resistance to diffusion is

$$r_a = U_r \;/\; U_*2$$

where r_a is aerodynamic resistance.

Friction velocity (U_*) is then estimated with the stability-corrected logarithmic windspeed profile relationship

$$\frac{U_r}{U_*} = \frac{1}{k}\left[\ln \frac{(z_r - d)}{z_0}\right](1 - \sigma\bar{R}_i)^{-1/2}$$

where z_r is reference height (cm), σ is an empirical constant (=10) and U_r is reference height windspeed. Zero plane displacement d = 0.63h where h is the height (cm) of the plant canopy, and roughness length (z_0) follows as

$$z_0 = k\ (h - d)$$

where k is Von Karman's constant (0.41).

continued...

Because the windspeed profile is affected by atmospheric stability, a mean Richardson Number is introduced

$$\bar{R}_i = \frac{gz\,(T - T_0)}{U_r^{\,2} T}$$

where g is the gravitational constant (cm² s⁻¹), T is reference height temperature (k), T_0 is the temperature of the surface losing heat (canopy temperature), U_r is reference height windspeed (cm s⁻¹), and z is height.

$$r_b = 0.12\left(\frac{1}{U_c}\right)^{1/2} D^{-2/3}$$

where D is the diffusivity of the gas and U_c is canopy windspeed. The characteristic length (l) is

$$l = \frac{4A}{P}$$

where A is planar area (cm²) of the leaf and P the perimeter (cm). A logarithmic profile is resumed in region 3 and the atmospheric resistance from z_c to zero ground displacement may be approximated by

$$r_c = U(z_c) \;/\; [U_*(z_c)^2]$$

Eddy velocity at z_c is

$$U(z_c) = U_h\, e^{-\alpha(1-z_c/h)}$$

where α is defined by the relationship

$$l_w = \frac{k}{\alpha}\left(h \;/\; \ln\left(\frac{h - d}{z_0}\right)\right)$$

The windspeed at canopy height h is then

$$U_h = \frac{U_*}{k}\ln\left(\frac{h - d}{z_0}\right)(1-\sigma\bar{R}_i)^{-1/2}$$

An estimate of the centre of the canopy layer is

$$z_c = h - \frac{l_w}{2}$$

The depth of the canopy eddy is $l_w = 0.473\ (h - d)$ and extends down from approximately h. Within this layer, friction velocity varies with height; therefore, at z_c

$$U_*(z_c) = U_* e^{-\alpha(1-z_c/h)}$$

$$SC_D = SC_{RT} \cdot I(phen)$$

$$f_{10} = F_{10} \cdot SC \cdot S_{RT}/S_{ROOT}$$

where SC_D is the determined shoot S/C ratio, SC_{RT} is the actual root S/C ratio, I(phen) is the predefined ratio of shoot S/C to root S/C as a function of phenology, f_{10} is the translocation rate from one root layer (g S m⁻² day⁻¹), F_{10} is the daily shoot carbon growth increment (g C m⁻² day⁻¹), S_{RT} is root sulphur in a layer, and S_{ROOT} is root sulphur summed over all layers (g S m⁻²).

continued...

If $NS_S \leq 35$

$$\text{then } y = MIN\ (1,\ 3.5 - 0.1 * NS_S)$$

$$\text{otherwise } y = 0$$

where y is the sulphur limiting effect on shoot photosynthesis and growth.

For sulphur-conserving shoot death,

$$CS_S = (CN_S + \delta) \cdot NS_S$$

$$f_{11} = (F_{11}/CS_S) - F_{11} \cdot \sigma/CS_{STS}$$

$$CS_{SM} = ((1-\sigma) \cdot F_{11}) / f_{11}$$

where CS_S is the C/S ratio of senescing shoots after conservation, CN_S is the C/N ratio of these shoots, δ is the increase in the C/N ratio in tissues where protein hydrolysis has occurred, σ is the fraction of structural shoot carbon, NS_S is the N/S ratio of the shoots, F_{11} is the total rate of flow of carbon due to shoot death (g C m^{-2} day^{-1}), f_{11} is total metabolic sulphur flow in dying shoots (g S m^{-2} day^{-1}), CS_{STS} is the shoot structural C/S ratio (fixed), and CS_{MS} is the C/S ratio of the dying metabolic components of dying shoots. Thus, structural sulphur in dying shoots is given by

$$f_{12} = (F_{11}/CS_S) - f_{11}$$

and total remobilization of sulphur by

$$f_{13} = F_{11} \cdot (1-\sigma) \cdot ((1/CS_{MDS}) - (1/CS_{MS}))$$

which is distributed among roots in all layers; CS_{MDS} is the C/S ratio of the metabolic component before protein hydrolysis.

Root sulphate uptake is calculated

$$U = V_{max} \cdot [SO_4]/(K_m + [SO_4])$$

$$f_9 = C_R \cdot E_R(T) \cdot E_R(W) \cdot E_U(CS_P) \cdot U$$

where U is the basic Michaelis-Menten uptake rate (g S m^{-2} day^{-1} g^{-1} root carbon), V_{max} is the maximum uptake rate, K_m the half-saturation constant, $[SO_4]$ is the concentration of sulphate in solution (ppm S), f_9 is the rate of uptake (g S m^{-2} day^{-1}), C_R is root carbon content (g C m^{-2}), $E_R(W)$ and $E_R(T)$ are the effects of water and temperature on root metabolism, and $E_U(CS_P)$ is the effect of the whole-plant S/C ratio on uptake.

Sulphate adsorption-desorption by soil is formulated by the Freundlich isotherm

$$\Delta S = b \cdot [SO_4]^{1/n}$$

where $[SO_4]$ is the concentration of sulphate solution (ppm S), ΔS is the quantity adsorbed (g S g^{-1} soil), and b and n are empirical constants.

The solubility product for the ions Ca^{2+} and SO_4^{2-} is used to determine gypsum precipitation

$$K_{SP} = [Ca^{2+}] \cdot [SO_4^{2-}] \cdot \gamma 2$$

where K_{SP} is the solubility product (2.4×10^{-5} at 25°C; and γ is the mean activity coefficient. When K_{SP} is reached, gypsum may precipitate. Although K_{SP} is actually temperature-dependent, this feature is not included in the model. The concentration of gypsum can be estimated

$$[CaSO_4] = [Ca^{2+}] \cdot [SO_4^{2-}] \cdot \gamma/K_D$$

continued...

where K_D is the dissociation constant (4.9×10^{-3}). The mean activity coefficient for the soil solution is estimated from

$$\ln \gamma = 0.509\ z^2 \sqrt{u} / (1 + \sqrt{u})$$

where z is the valence of the ion and u is its ionic strength, given by

$$u = 1/2 \sum_{i=1}^{n} C_i z_i$$

where C_i is the concentration of one of the n ions in solution. The ions considered here include Na^+, K^+, Ca^{2+}, Mg^{2+}, and SO_4^{2-}.

Diffusion of sulphate is described by Fick's law, where the diffusion rate is proportional to the concentration gradient. Thus,

$$D_f = D \cdot (\Delta\ [SO_4] / \Delta\ X) \cdot \theta$$

where D_f is the diffusion rate (g S cm^{-2} day^{-1}), $\Delta\ [SO_4]$ is the concentration difference between layers, $\Delta\ X$ is the distance (cm) between the midpoints of adjacent layers, D is diffusivity (cm^2 day^{-1}), and θ is the volumetric soil water content, necessary here to express diffusion rate per cross-sectional area of soil.

The rate of sulphate uptake is then modified by the effects of soil water content and temperature on general microbial metabolism, and by the demand for sulphur as expressed in the microbial C/S ratio

$$a_3 = E_m(T) \cdot E_m(W) \cdot E_u(CS_m)$$

and

$$f_3 = a_3 \cdot C_m \cdot V_{max} \cdot [SO_4] / (K_m + [SO_4])$$

where a_3 is the combined effect of temperature $E_m(T)$, water $E_m(W)$, and C/S ratio ($E_u(CS_m)$). V_{max} is the maximum uptake rate, $[SO_4]$ is the concentration of sulphate in soil solution (ppm S), C_m is the microbial biomass (g C m^{-2}), and K_m is the half-saturation constant.

In the model, mineralization and sulphate uptake are affected by the same functions of temperature and moisture. The model also includes a microbial C/S effect, that mirrors the effect of the C/S effect on sulphate uptake, given by

$$a_4 = E_m(T) \cdot E_m(W) \cdot E_{mn}(CS_m)$$

$$f_4 = a_4 \cdot S_m \cdot V_{max}$$

where $E_m(T)$ and $E_m(W)$ are as in Eq. [4] (Coughenour 1981), $E_{mn}(CSm)$ is the effect of the C/S ratio, a_4 is the combination of these effects, f_4 is the mineralization rate (g S m^{-2} day^{-1}), V_{max} is the maximum uptake rate (day^{-1}), and S_m is microbial sulphur content (g S m^{-2}). Maximum rates were chosen as 0.8 day^{-1} for bacteria and 0.165 day^{-1} for fungi.

The oxidation of sulphide to sulphate is controlled by soil aeration and bacterial metabolism. Bacterial metabolism is expressed as a function of temperature and soil water content. The oxidation relationship is

$$a_5 = E_m(T) \cdot E_m(W) \cdot E_{ox}(W)$$

$$f_5 = a_5 \cdot V_{ox} \cdot S_r$$

where $E_m(T)$ and $E_m(W)$ are the effects of temperature and water on the bacteria, $E_{ox}(W)$ is the effect of water on aeration, a_5 is the combined effect, f_5 the oxidation rate (g S m^2 day^{-1}), S_r is the quantity of reduced forms of sulphur (g S m^{-2}),

continued...

and V_{ox} is the maximum oxidation rate (day^{-1}) based on results from a silt loam soil in which 55% of the reduced sulphur was oxidized in three weeks. Thus, this expression assumes that the rate of oxidation is proportional to S_r.

The rate of volatilization of sulphur during decomposition is represented as a proportion of the rate of decomposition of metabolic litter, increasing slightly as aeration declines

$$f_6 = F_6 \cdot P_V(W) \cdot SC_{me}$$

where f_6 is the volatilization rate (g S m^{-2} day^{-1}), F_6 is the rate of metabolic litter decomposition (g C m^{-2} day^{-1}), $P_V(W)$ is the variable proportion of F_6 as a function of soil water based on data of Banwart and Bremner (1976) as cited by Coughenour (1981), and SC_{me} is the S/C ratio of metabolic litter. We assume that this equation applies to all soil layers.

Sulphate esters are not explicitly treated, because of the uncertainty of their origin, but are assumed to be associated with humads and resistant soil organic matter. A regression equation, based on the data of Cooper (1972) and Bettany et al. (1973, 1974) as cited by Coughenour (1981), predicts that HI-sulphur (S_{HI}, g S m^{-2}) is a function of total sulphur (S_{total}, g S m^{-2}) and total carbon (C_{total}, g C m^{-2})

$$S_{HI} = 0.71 \cdot S_{total} - 0.0029 \cdot C_{total}$$

This equation can be used to calculate HI sulphur at any point in the simulation.

When microbial death is calculated in the decomposer submodel, sulphur flow is controlled by carbon flow. Thus

$$f_1 = F_1 / CS_{stm}$$

where f_1 and F_1 are the flows (g m^{-2} day^{-1}), respectively, of structural sulphur and structural carbon due to death, and CS_{stm} is the fixed C/S ratio of the microbial structural component.

The flow from metabolic components varies with the C/S ratios of the microbes, as

$$f_2 = (F_2 / CS_m) - f_1$$

where f_2 and F_2 are the flows of metabolic sulphur and metabolic carbon due to death, and CS_m is the C/S ratio of the microbes.

$$f_7 = RS \cdot \beta \cdot \alpha$$

$$f_8 = R_S \cdot \beta \cdot (1 - \alpha)$$

where f_7 is the rate of sulphate release from humads (g S m^{-2} day^{-1}), and f_8 is the rate of release from resistant organic material (g S m^{-2} day^{-1}).

$$\alpha = \lambda \cdot S_h / (\lambda \cdot S_h + S_{re})$$

$$\alpha = SC_h/SC_{re}$$

where λ is the lability of humad-associated esters compared to that of resistant organic-associated esters, SC_h and SC_{re} are, respectively, the S/C ratios of humads and resistant organic material, α is the proportion of sulphate originating from humads, S_h is humad sulphur content (g S m^{-2}), S_{re} is resistant organic sulphur (g S m^{-2}).

If B_0 is the sum of root and microbial biomasses per cm^3 of soil in the surface layer, and B_1 is the equivalent measure in a deeper layer, then

$$\beta = B_1 / B_0$$

is the proportional decrease in activity for layer 1.

continued...

Flow of S uptake by nematodes:

$$f_{ni} = Ic/46$$

Flow of S excreted by nematodes and to metabolic litter

$$f_{no\ ml} = 0.25\ E/46$$

Flow of S excreted by nematodes and to structural litter

$$f_{no\ sl} = 0.75\ E/46$$

The first approximation to intake is

$$I_c = M_r(T) \cdot 0.02925$$

where I_c is the intake rate (g C g^{-1} nematode C day^{-1}), $M_r(T)$ is the temperature-dependent metabolic rate (ml O_2 g^{-1} fwt h^{-1}), and feces production $E = I_c \cdot (1-AE)$. AE is assimilation efficiency (0.5).

Kercher, J.R. 1977. GROW1: a crop growth model for assessing impacts of gaseous pollutants from geothermal technologies. UCRL-52247. Lawrence Livermore Laboratory, Livermore, California.

List of Symbols

Symbols	Description	Value Used In Examples
a_L	Conversion factor for changing LAI to leaf dry weight (g/m^2)	33
a_1	Coefficient determining translocation of photosynthate	1
a_4	Coefficient determining amount of storage to be held in reserve (g)	1
A_0	Total concentration of PGA and RuDP (mol/L)	see k3
A	Ratio of total root-surface area to area of ground	
b_1	Coefficient determining translocation of photosynthate	1
b_4	Parameter determining slope of function that cuts off flow of photosynthate out of main storage as main storage level approaches a critical value	0.1
B_c	Converts g CO_2 cm^{-2} s^{-1} to g dry wt m^{-2} da^{-1}	4.69×10^8
c_1	Reduction in photosynthesis for unit increase in pollutant with one unit of diffusion resistance (s cm^{-1} ppm^{-1})	0.7125
c_2	Inverse slope of function cutting off flow of photosynthate from leaf storage to structural leaf as $x2/x1 \to 0$	0.05
C_a	Concentration of CO_2 in air (g/cm^3)	310 ppm
C_c	Concentration of CO_2 at chloroplast (g/cm^3)	
C_{ia}	Concentration of CO_2 in pore (g/cm^3)	
C_p	Concentration of CO_2 in protoplasm (g/cm^3)	
C_{soil}	Concentration of salts in soil (mol/cm^3)	0
d	Inverse of square of standard deviation of foliage density (m^{-2})	
d_7	Thickness of rooting zone layer in soil (m^{-1})	
d_8	Thickness of surface zone layer of soil (m^{-1})	
D	Diffusivity in the canopy (cm^2/s)	
D_d	Time of dawn (da)	
D_L	Leaf width (cm)	7
D_0	Turbulent diffusivity in air (cm^2/s)	300
D_s	Time of sunset (da)	

continued...

Symbols	Description	Value Used In Examples
e	Vapour pressure (mbar)	
e_s	Saturation-vapour pressure (mbar)	
e_1	Leaf-growth constant (da^{-1})	0.137
e_4	Growth constant for stem and fruit (da^{-1})	2.44
e_6	Growth constant for root (da^{-1})	0.15
ET	Evapotranspiration (m/da)	
$f(Z)$	Density of leaves in the canopy as a function of Z	
$f_L(\alpha)$	Angular distribution of leaves	
F	Leaf area index LAI (area of leaves/area of ground)	
F_O	Maximum allowed LAI in simulation	5.6
F_{TOT}	Total LAI	
G_i	Net flux of radiant energy out of layer i in the downward direction (cal cm^{-2} s^{-1})	
h'	Ratio of F_{TOT} to total canopy depth Z_{TOT} (cm^{-1})	0.025
H	Unit step function (Heaviside function); rate of sensible heat transfer from the leaf	
I	Flux of light or light intensity normal to the leaf at canopy depth F (nanoeinstens cm^{-2} s^{-1} or cal cm^{-2} s^{-1})	
I_L	Light flux reaching F from the direction of the sun	
I_m	Light intensity at photosynthesis half maximum	
I_n	Net radiation into the canopy (cal cm^{-2} s^{-1})	
I_O	Light flux at top of canopy in the direction of the sun (cal cm^{-2} s^{-1})	.02
k_1	Equilibrium constant for conversion of CO_2 and RuDP to PGA (cm^3/g)	2.28×10^8
k_2	Equilibrium constant for light conversion of NADP to NADPH (cm^2 s/cal or cm^2 s/μeinsteins)	21.9 cm^2 s cal^{-1}
k_3	Coefficient for maximum photosynthesis for high CO_2 and high light (g cm^{-2} s^{-1} $mole^{-2}L^2$)	$k_3A_ON_O$ = 500 mg dm^{-2} h^{-1}
k_d	Relative rate of growth during day	1
k_n	Relative rate of growth during night	1
k	Decay constant for reduction of windspeed in canopy	0.44
K_{soil}	Maximum value of soil hydraulic conductivity (weight basis, m/da)	

continued...

Symbols	Description	Value Used In Examples
$K_{(xi)}$	Hydraulic conductivity of the soil (m/da)	
K	Extinction coefficient of light in the canopy	
L	Number of layers in canopy	10
M_d	Number of plants per unit area (m^{-2})	5
$\hat{n}$	Normal to the plane of the leaf	
N_o	Total concentration of NADP and NADPH (mol/L)	see k3
P	Photosynthesis (g cm^{-2} s^{-1})	
P_g	Gross photosynthesis (g cm^{-2} s^{-1})	
P_m	Maximum values of photosynthesis at high light levels	
P_n	Net photosynthesis	
P_r	Precipitation (m/da)	
P_1	Precipitation intercepted by leaves (m/da)	
P_2	Precipitation striking ground without interception (m/da)	
PL	Average cosine of projection of sunlight onto leaf for all leaves	
$PL\alpha$	Average cosine of projection of sunlight onto leaves at angle α	
Q_{10}	Ratio of respiration at $(T_x + 10)$°K to respiration at T_x °K, where T_x is a reference temperature	2
r_a	Leaf-boundary-layer resistance (s/cm)	
r_c	Carboxylation resistance	
r_{ci}	Turbulent diffusion resistance from canopy layer i to top of canopy (s/cm)	
r_{cw}	Cell-wall-diffusion resistance (s/cm)	0.126
r_g	Specific growth-respiration rate	0.35 at 25°C
r_I	Stomatal resistance due to all factors except water stress (s/cm)	
r_m	Mesophyll-cell resistance (s/cm)	
r_n	Specific maintenance-respiration rate	0.006 at 25°C
r_p	Protoplasm resistance to CO_2 diffusion (s/cm)	1.0
r_s	Stomatal-diffusion resistance (s/cm)	
r_{soil}	Resistance to hydraulic flow of water in the soil (da, weight basis)	

continued...

Symbols	Description	Value Used In Examples
r_{sp}	Resistance to flow of water between soil and the plant (da, weight basis)	
r_{w1}	Parameter proportional to slope of curve of stomatal resistance as a function of water stress (soil-water potential) (bar s cm^{-1})	5.004
r_{w2}	Value of ψ_s at which stomatal resistance is singular (bar)	-15
r_{w3}	Soil-water potential at a soil-water content of 0 (bar)	-267
r_{w4}	Logarithm of the ratio of the soil-water potentials with one unit of soil-water-content difference between them (m^{-1})	85.67
r_o	Critical or maximum stomatal resistance attained when ψ_{Li} is maximum	
r_1	Leaf-boundary-layer resistance when D_L = 1 cm and U = 1 cm/s (s/cm)	1.3
R	Respiration (usually leaf) (g cm^{-2} s^{-1})	
R_G	Gas constant (bars $°K^{-1}$ mol^{-1} cm^3, or cal mol^{-1} $°K^{-1}$)	8.314 J mol^{-1} $°K^{-1}$
R_x	Dark leaf respiration at 25°C (g cm^{-2} s^{-1})	2.5 mg dm^{-2} h^{-1}
$\hat{s}$	Unit vector in direction of the sun	
s	Absorption coefficient of CO_2 in water	0.756 at 25°C
S	Air-pollutant concentration (ppm)	
S_o	Threshold for depressant effect of pollutant (ppm)	20 pphm
S_L	Ratio of leaf storage to leaf structural tissue at which photosynthesis is at half maximum	
S_p	Reserve concentration of leaf storage photosynthate that the leaf retains	0.1
t	Time (da)	
T	Temperature, usually of air (°K)	
T_i	Transfer flux to compartment i from storage (g m^{-2} d^{-1})	
T_r	Root or soil temperature (°K)	
T_{rns}	Transfer coefficient for movement between leaf storage and main storage (da^{-1})	3.0
T_x	Reference temperature for calculating respiration (°K)	25°C
u	Inverse of exponent that transforms soil content to soil potential	
u_1	Inverse of max$[P_n(I)]/C_a$ at high light levels (ppm g^{-1} cm^2 s)	

continued...

Symbols	Description	Value Used In Examples
U	Windspeed (cm/s)	
v	Exponent of soil potential used to calculate soil conductivity from soil potential	
v_1	Inverse of slope of $P_n(I)$ at low light levels (nanoeinsteins/g)	
w	Value of soil potential at which soil conductivity has fallen to half maximum (m)	
w_1	Inverse of slope of $P_g(I)$ at low light levels (nanoeinsteins/g)	
x_1	Biomass (dry wt) of structural leaf material (g)	
x_2	Biomass (dry wt) of leaf material in storage (g)	
x_3	Biomass (dry wt) of main storage (g)	
x_4	Stem biomass (dry wt) (g)	
x_5	Fruit biomass (dry wt) (g)	
x_6	Root biomass (dry wt) (g)	
x_7	Soil water in the root zone (m)	
x_8	Soil water in the soil-surface zone (m)	
x_9	Water in the leaf-interception storage (m)	
x_{7max}	Maximum water content of the root zone (m)	0.12
Z	Vertical distance usually measured from the top of the canopy (m)	
Z_{TOT}	Thickness of the canopy (m)	
α	Angle of the leaf to the horizon	
β	Elevation of the sun	
γ	Psychometric constant (mbar/°K)	0.66
δ	Angle between the sun and the leaf	
Δ	Derivative of saturation vapour pressure with respect to temperature (mbar/°K)	
η	Angle between the sun and the normal to the leaf	
θ	Volumetric water content at which matrix potential is equivalent to a pressure of 1 m of water	
λ	Latent heat of vaporization (cal/g)	558
μ	Power of x_4 used to calculate biomass of x_4 capable of growth	1.0
μ_1	Coefficient proportional to slope of $r_s(I)$ (s^2 cm cal^{-1})	1.3×10^{-3}

continued...

Symbols	Description	Value Used In Examples
μ_2	Coefficient inversely proportional to square root of slope of $r_s(I)$ at I = 0 (nanoeinsteins cm^{-2} s^{-1} or cal cm^{-2} s^{-1})	3.33 x 15^{-6} cal cm^{-2} s^{-1}
μ_3	Slope of rs(T) (s cm^{-1} $^oK^{-1}$)	0.5
μ_4	r_s at 0.0°C, infinite light levels, and no water stress (s/cm)	-7.0
ν	Water-stress component to stomatal resistance	
ξ_1	Relative growth constant for stem	2.0
ξ_2	Relative growth constant for fruit	0.0346
ρ_{Ls}	Saturation concentration of water vapour at the leaf	
ρ_Z	Concentration of water vapour at reference height Z	
ρc	Volume heat capacity of air (cal cm^{-3} $^oK^{-1}$)	290 x 10^6
σ	Function of α and β used in calculating PL_α	
τ_0	Physiological time for initiation of fruit growth (degree-da)	800
τ_1	Physiological time for termination of fruit growth (degree-da)	2500
ψ_c	Critical water potential at which r_s attains its maximum value (m, weight basis)	
ψ_s	Soil-water potential (bars)	
ψ_{Li}	Leaf potential for layer i (m, weight basis)	
ψ_7	Soil-water potential for root-zone layer (m, weight basis)	
ψ_8	Soil-water potential for soil-surface layer (m, weight basis)	
ω	Azimuthal angle between sun and leaf	

continued...

We define growth as the transfer of photosynthate from a storage compartment (x_2 leaf storage or x_3 main storage) to a structural compartment (x_1 leaf, x_4 stem, x_5 fruit, or x_6 root).

The equations describing the rate of change of the state variables x_1 through x_6 with time are described mathematically as:

$$\frac{dx_1}{dt} = T_1,$$

$$\frac{dx_2}{dt} = \frac{S_L P_T H(P_T)}{S_L + x_2/x_1} + H(-P_T)P_T - [1 + r_g(T)]T_1 - T_3 - r_n(T)x_2,$$

$$\frac{dx_3}{dt} = T_3 - (1+r_g)(T_4+T_5+T_6) - r_n(T_r)x_6 - r_n(T)(x_3+x_4+x_5),$$

$$\frac{dx_4}{dt} = T_4 - r_n(T)x_4\ H(a_4 x_4{}^{\mu} - x_3),$$

$$\frac{dx_5}{dt} = T_5 - r_n(T)x_5\ H(a_4 x_4{}^{\mu} - x_3),$$

and

$$\frac{dx_6}{dt} = T_6 - r_n(Tr)x_6\ H(a_4 x_4{}^{\mu} - x_3),$$

where

$$P_T = B_c \int_0^F P_p(F)\ dF/M_d,$$

$r_g(T)$ = growth-respiration rate with a dependence on T as R above,
$r_n(T)$ = maintenance-respiration rate with a dependence on T as R above,
T = temperature of above-ground parts (°K),
T_r = temperature of roots (°K),
μ = exponent of x_4 for calculating the fraction of x_4 used in growth,
a_4 = empirical parameter,
S_L = ratio of leaf storage to leaf structural tissue at which photosynthesis is at half its maximum value,
P_T = added biomass (g dry wt da^{-1} $plant^{-1}$),
B_c = conversion factor from g CO_2 cm^{-2} s^{-1} to g dry wt m^{-2} da^{-1} (4.69 x 10^8), and
T_i = transfer flux to compartment i, i=1,3,4,5,6.

$$T_1 = e_1 x_1\{k_n[H(D_d - t) + H(T - D_s)] + k_d H(t - D_d)\ H(D_s - t)\} \frac{x_2/x_1}{c_2 + x_2/x_1} (1 - M_d x_1/a_L F_0),$$

$$T_3 = T_{rns}\ x_2 \left(\frac{a_1 x_2}{x_1 + x_2} - \frac{b_1 x_3}{x_3 + x_4 + x_5 + x_6}\right) H\left(\frac{x_2}{x_1 + x_2} - S_p\right),$$

continued...

$$T_4 = e_4 \xi_1 x_4^{\mu} H(x_3 - a_4 x_4) \frac{x_3 - a_4 x_4^{\mu}}{b_4 + x_3 - a_4 x_4^{\mu}} ,$$

$$T_5 = H(\tau - \tau_0) e_4 \xi_2 x_5 H(x_3 - a_4 x_4^{\mu}) H(\tau_1 - \tau) ,$$

and

$$T_6 = e_6 x_6 \frac{x_3 - a_4 x_4^{\mu}}{b_4 + x_3 - a_4 x_4^{\mu}} H(x_3 - a_4 x_4^{\mu}) .$$

$$P_p = P_n \left[1 + \frac{c_1}{r_s} \left(S_o \frac{r_s}{r_b} - S \right) \right] , \qquad S > S_o ,$$

$$= P_n \left[1 + \frac{c_1}{r_s^{\,2}} \frac{S\, r_b}{S_o} \left(S_o \frac{r_s}{r_b} - S \right) \right] , \quad 0 < S < S_o$$

where

c_1 = reduction in photosynthesis for a unit increase in pollutant at one unit of diffusion resistance, ($s\ cm^{-1}\ ppm^{-1}$),
r_s = stomatal resistance (s/cm),
S = concentration of pollutant (ppm), and
r_b = stomatal resistance at which S_o was determined.

$$P_n = \frac{-b - \sqrt{b^2 - 4ac}}{2a} - R ,$$

where

$$a = (k_2 I + 1)\, k_1 [r_p + r_{cw} + s(r_s + r_a)],$$

$$b = -(k_2 I + 1) \{ s C_a k_1 + R k_1 [r_{cw} + s(r_s + r_a)] + 1 \}$$

$$- k_1 k_2 k_3 A_o N_o I [r_p + r_{cw} + s(r_s + r_a)] , \text{ and}$$

$$c = k_1 k_2 k_3 A_o N_o I \{ R [r_{cw} + s(r_s + r_a)] + s C_a \} .$$

Following Sinclair, we use for r_a and r_s:

$$ra = r_1 (D_L / U)^{1/2},$$

where D_L = leaf width, U = windspeed, and r_1 is a constant, and

$$r_s = \frac{\mu_1}{I + \mu_2} + \mu_3 T + \mu_4 + \upsilon,$$

where μ_1, μ_2, μ_3, and μ_4 are constants determined by fitting $r_s(I,T)$ to data obtained by varying light intensity and leaf temperature while measuring r_s · μ_1 is in units of either nanoeinsteins cm^{-3} or cal cm^{-3}, μ_2 in either nanoeinsteins $cm^{-2}\ s^{-1}$ or cal $cm^{-2}\ s^{-1}$, μ_3 in s $cm^{-1}\ C^{-1}$, and μ_4 in s cm^{-1}. υ is a water stress term to be discussed below. The biochemical constants, k_1, k_2, k_3, A_o, and N_o can be easily determined by examining Eq. [21] in Kercher 1977 at various limits and using experimental data to fit the equation at these limits (see Sinclair in Kercher 1977 for a full discussion). Our expression for respiration is that of Waggoner:

continued...

$$R = R_x \exp[T_x(T_x + 10) \ln Q_{10}(1/T_x - 1/T)/10] ,$$

where

R_x = base respiration rate,
T_x = base temperature (°K), and
Q_{10} = ratio of $R(T_x + 10)$ to $R(T_x)$.

$$\frac{dx_7}{dt} = \frac{\psi_8 - \psi_7}{r_{soil}} H(x_{7max} - x_7) - \sum_i \frac{\psi_7 - \psi_{Li}}{r_{sp}} ,$$

$$\frac{dx_8}{dt} = [P_2 + P_1 H(x_9 - x_{9max})] H(x_{8max} - x_8) - \frac{\psi_8 - \psi_7}{r_{soil}} - ET(G,0,T,e,0,r_{gnd}) ,$$

$$\frac{dx_9}{dt} = P_1 H(x_{9max} - x_9) - \sum_{\substack{\text{canopy} \\ \text{layers} \\ i = 1}}^{L} ET(In_i, In_{i+1}, T, e, 0, r_{ai}' + r_{ci}') .$$

ψ_8 = soil-water potential of surface-soil water (m),
ψ_7 = soil-water potential of rooting-zone water (m),
ψ_{Li} = leaf-water potential of leaves in layer i (m),
r_{soil} = resistance of soil to water flow (da),
r_{sp} = resistance to flow between soil and plant leaves (da),
P_2 = precipitation striking ground without interception (m/da), and
P_1 = precipitation intercepted by leaves (m/da).

$$\frac{\psi_7 - \psi_{Li}}{r_{sp}} = ET\ (In_i,\ In_{i+1},\ T,\ E,\ r_{si}',\ r_{ai}' + r_{ci}') .$$

Stomatal resistance (of H_2O) of the i^{th} foliage layer is given by

$$r_{si}' = r_{Ii}' + (r_o - r_{Ii}')\, e^{(\psi_c - \psi_{Li})^m} ,$$

where

r_o = critical or maximum resistance attained when $\psi_{Li} = \psi_c$(s/cm)
ψ_c = critical potential (mbar), and
m = slope of resistance with respect to change in ψ_{Li} at ψ_c (mbar^{-1}).

$$r_{ci} = \frac{1}{D_o K_\alpha h'} (e^{k_\alpha h' Z} - 1) .$$

$$r_{soil} = \frac{d_8}{2K(x_8)} + \frac{d_7}{2K(x_7)} ,$$

and

$$r_{sp} = \frac{d_7}{2K_r} + \frac{d_7\ \delta}{fK(x_7)A} ,$$

continued...

where

d_i = thickness of soil layer i (m),
δ = ratio of cross-sectional area of roots in x_7 to area of x_7,
f = fraction of root surface area through which water is absorbed,
A = ratio of total root surface area to area of ground,
K_r = conductivity of plant tissue (m/da);

and we calculate soil potentials using

$$\psi_7 = d_8 + \frac{d_7}{2} + \left(\frac{\theta d_7}{x_7}\right)^{1/u},$$

and

$$\psi_8 = \frac{d_8}{2} + \left(\frac{\theta d_8}{x_8}\right)^{1/u}$$

Soil conductivities are calculated, using

$$K(x_i) = \frac{K_{soil}}{\left(\frac{\psi_i}{w}\right)^{v} + 1},$$

where v and u are empirical constants easily determined by log-log fits of soil water potential versus soil water content and

K_{soil} = soil conductivity at soil potential equal to 0,
θ = volumetric water content at which matric potential is equivalent to a pressure of 1 m of water, and
w = value of soil potential at which soil conductivity has fallen to half maximum.

$$\frac{dx_7}{dt} = P_r\ H(x_{7max} - x_7) - \sum_{i=1}^{L} ET(I_{ni}, G_i, T_i, e, r_{si}', r_{ai}' + r_{ci}'),$$

where

I_{ni} = total incident radiant energy into layer i (cal cm^{-2} s^{-1}),
G_i = total incident radiant energy emerging from layer i (cal cm^{-2} s^{-1}),
T_i = temperature of layer i,
e = vapour pressure of atmosphere above the canopy (mbar),
r_{si}' = stomatal resistance of layer i,
r_{ai}' = boundary layer resistance of leaves in layer i,
r_{ci}' = canopy-diffusion resistance from layer i to a reference level where e is measured,
P_r = precipitation rate (m/da), and
$H(x)$ = 1, $x > 0$
= 0, $x < 0$.

$$r_s' = r_I' + \nu'.$$

Curry gives ν' as a function of soil-water potential ψ_s.

$$\nu' = \frac{r_{w1}}{r_{w2} + \psi_s(x_7, C_s)} - \frac{r_{w1}}{r_{w2} + \psi_s(x_{7max}, 0)}$$

where the soil-water potential is a function of soil-water content and soil salt concentration.

continued...

$$\psi_s(x_7, C_{soil}) = -r_{w3} e^{-r_{w4} x_7} - R_G T_r C_{soil},$$

where

R_G = gas constant (83.14×10^3 mbar cm³ mol⁻¹ °K⁻¹),
T_r = temperature of soil (°K), and
C_{soil} = concentration of salt in soil (mol cm⁻³ solute).

$$ET = \frac{\Delta(I_n - G) + \rho c[e_s(T) - e] / (r_a' + r_c')}{\lambda\{\Delta + \gamma\ [1 + r_s'/(r_a' + r_c')]\}}\ 864\ ,$$

where

ET = transpiration (m/da),
$e_s(T)$ = saturation vapour pressure at temperature T (mbar),
ρc = volume heat capacity of dry air (290×10^{-6} cal cm⁻³ °K⁻¹),
γ = psychometric constant (0.66 mbar °K⁻¹),
λ = latent heat of evaporation (585 cal/g),
Δ = de_s/dT;

and $e_s(T)$ and Δ are calculated by the computer code using the Clausius-Clapeyron equation.

Kercher, J.R. and M.C. Axelrod. 1981. SILVA: a model for forecasting the effects of SO_2 pollution on growth and succession in a western coniferous forest. UCRL-53109, Lawrence Livermore National Laboratory, Livermore, CA. 72 pp.

$$H = 137 + b_2D - b_3D^2,$$

where b_2 and b_3 are constants.

$$\delta D = \frac{G\ D\ [1 - (DH)/(D_mH_m)]}{274 + 3b_2D - 4b_3D^2}\ r(A)\ Q(DEGD)\ S(BAR)\ W(_\tau)\ GR$$

where:

a	= growth constant for each species at the optimum site (cm y^{-1})
L	= leaf area of tree (cm^2)
D	= diameter of tree (dbh in cm)
H	= height of tree (cm)
H_m	= maximum height species attains
D_m	= maximum dbh species attains
r	= response to light (dimensionless)
A	= available light at tree
Q	= response to climate (dimensionless)
DEGD	= growing degree days (F-days)
S	= response to soil quality (dimensionless)
BAR	= total basal area of stand (cm^2)
W	= response to water stress (dimensionless)
τ	= ratio of actual to potential evapotranspiration
GR	= response to pollution

$$A = A_0\ e(-\kappa \sum_i\ LAI)$$

where κ is an extinction coefficient for coniferous canopies, LAI is the leaf area index, and the sum is over all trees taller than the tree under consideration. A_0 is the light at full sunlight. The constant κ is taken to be 0.47.

$$\Sigma LAI = (\Sigma L)/PLTSIZ$$

where PLTSIZ is the ground area of the plot.

$$r(A) = 1 - e^{[-4.64\ (A-0.05)]},\ \text{shade tolerant}$$

$$= 2.24\{1 - e^{[-1.136(A-0.08)]}\},\ \text{shade intolerant.}$$

The leaf area of each tree as a function of tree diameter is given by:

$$L = c_i D^{\alpha_i}$$

where c_i and α_i are constants determined for each species for logarithmic regressions. Usually α_i lies between 1.5 and 2.5.

$$Q = 4\ (DEGD - DMIN)\ (DMAX - DEGD)/(DMAX - DMIN)^2$$

$$DEGD = \int_{\text{growing season}} (T - 40)\ B(T - 40)\ dt$$

where T is the temperature in Fahrenheit, and B(T - 40) is 1 for T greater than 40 and 0 for T less than 40.

$$S(BAR) = 1 - BAR/(SOILQ \cdot 10{,}000 \cdot PLTSIZ)$$

continued...

where BAR = total basal area of all species on stand. The parameter SOILQ is the maximum basal area which the plot can carry and is dimensionless (m^2/m^2). This parameter is determined by soil nutrients. The factor of 10,000 converts cm^2 of BAR to m^2. The function S reduces growth for all trees as the total basal area approaches the maximum allowed.

$$W(\tau) = 1 - \left(\frac{WSM - \tau}{WSM - WSO}\right)^{NWS}$$

to quantify W, where

τ = annual actual evapotranspiration / annual potential evapotranspiration
WSM = value of τ at which W is maximum
WSO = lower limit of range of tolerance in τ
NWS = exponent relating linear function of τ to tree response.

Average overall M age classes to get the total response of the tree:

$$GR = \sum_{k=1}^{M} w_k GR_k$$

where w_k = weight of each needle age class to total productivity.

Let GRP_k (SA_j) be the response of the productive capacity of the k^{th} year needles to fumigations during the j^{th} year. The current year is 1; last year is 2; etc. Then the accumulated effect of all fumigations on the k^{th} year needles is given by either:

$$GR_k = GRP_k\left(\sum_{j=1}^{k} SA_j\right)$$

or

$$GR_k = \left(\prod_{j=1}^{k}\right) GRP_k(SA_j).$$

SA = seasonal average concentration (ppm).

$$GRP_k(SA_j) = 1 - PL\ (SA_j - CR)$$

CR = threshold concentration for growth reduction (ppm).
PL = fraction growth potential lost per ppm of SO_2 (ppm^{-1}).

PL and CR vary from species to species.

For a series of successive episodes during a growing season, it is necessary to assume that the concentration y_i and duration t_i for each episode are known. The accumulated effect of all fumigations on the k^{th}-year needles is given by

$$GR_k = GRP_k\left(\sum_{ji} \int^{q} y_j\ dt\right)$$

or

$$GR_k = GRP_k\left(\sum_{ji}^{q} y_{ij}\ \Delta t_{ij}\right)$$

Equation 31a or 31b is used in Equation 19 (Kercher 1977) to get the total growth response by averaging over all M needle-year classes.

continued...

The response of the productive capacity of the k^{th}-year needles to the N episodes during the j^{th} year is given by

$$GRP_k\left(\sum_i^N \int^q y_j dt\right) = 1 - \phi \quad \frac{1}{q} \ln \sum_i^N \int^q y\,(t;_{\nu ij,\omega ij})dt - \ln m_g \;/\; \ln s_g$$

or

$$GRP_k \sum_i^N {}^q\, y_{ij}\Delta t_{ij} = 1 - \phi \quad \frac{1}{q}\ln \sum_i^N {}^q\, y_{ij}\Delta t_{ij} - \ln m_g \,/\ln s_g$$

where in Equation 30b (Kercher and Axelrod 1981),

Δt_{ij} = the duration of the i^{th} episode in the j^{th} year, and
y_{ij} = the concentration of SO_2 in the i^{th} episode in the j^{th} year, depending on the pollutant episode data set.

The ϕ refers to the fractional loss of the productivity of the plant in the presence of pollution compared to productivity in the absence of pollution.

m_g, s_g, and q are parameters determined by fitting data.

The parameter ν is a measure of the skewness of the pulse. For ν near 1, the pulse is maximally skewed; as ν increases, the pulse becomes more symmetric.

The parameter ω is the width of the pulse.

Only establish seedlings for species i if the condition

$$DMIN(i) < DEGD < DMAX(i)$$

is satisfied. Total number of trees of each species J added to the plot is

$$N(J) = SDLINGS(J) \cdot P_S.$$

$$P = \frac{J}{J(1 - h) + N}$$

where

P = probability of a successful seed production year,
J = number of successful seed production years in a sequence of N years,
h = 1 + number of blocked years following a successful seed crop year for the species.

10 seedlings established per (10m x 10m) plot (SDLINGS) for each species for its good seed year.

As a first order approximation for the effects of shade on seedling survival of species intolerant to heat and moisture stress,

$P_S(I)$ = probability of survival (moisture-stress intolerant)

$= 1 - e^{(-\gamma_1\ LAI)}$.

On the other hand, some species are adapted to exposed sites, are shade intolerant, and exhibit increased mortality under shade as seedlings. For these species

$P_S(T)$ = probability of survival (moisture-stress tolerant)

$= e^{(-\gamma_2\ LAI)}$.

A quantitative fit for γ_1 and γ_2 was not possible from the available data in the above references. The authors have hypothesized the value 1.0 for both γ_1 and γ_2 because of the qualitative descriptions in the above references.

continued...

$$PD_T = PD_E + PD_G - PD_E PD_G$$

where the T, E, and G subscripts refer to total, ecological, and growth-suppressed, respectively, and

PD_T = probability of single tree death during year
PD_G = 0.369
PD_E = 4/AGEMX.

King, D.A., J.R. Kercher, and G.E. Bingham. 1983. Modeling the effects of air pollutants on soybean yield. In: Analysis of Ecological Systems: State-of-the-art in Ecological Modelling, eds. W.K. Lauenroth, G.V. Skogerboe, and M. Flug. New York: Elsevier Scientific Publishing, pp. 545-555.

The change in photosynthetic capacity F, caused by a pollutant acting on that component with turnover time d^{-1}.

$$\frac{df}{dt} = B(I,E) - (d + I)F$$

where

F = factor multiplying leaf photosynthesis
I = internal concentration of phytoactive agent
B = regeneration rate of F
E = available energy for regeneration.

The function B and rate d are hard to measure. For small turnover and repair rates and chronic fumigations, a simple approximate solution to Eq. 1 is given by

$$F = 1 - a \int_0^t I dt$$

where

a = constant determined from photosynthesis measurements,
I = internal concentration of phytoactive agent.

Assuming that internal loss of toxic agent is proportional to its concentration and the agent is replenished by diffusion into the leaf, then Eq. 2 may be rewritten

$$F = 1 - a' \int_0^t \frac{[O_3(t)]}{r(t) + b} dt$$

where

r = sum of resistance to O_3 diffusion
$[O_3]$ = external ozone concentration (time dependent)
a'; b = constants determined from photosynthesis measurements.

Mortensen, P. 1984. Modelling ion uptake in agricultural crops. RISO-M-2446. Riso National Laboratory, Roskilde, Denmark. 33 pp.

Calculation of the total concentration of an ion is:

$$CC = CC_0 + \frac{C_{in} + C_{out}}{BM} \quad (mol \cdot kg(DW)^{-1})$$

where

CC_0 is the concentration of an ion at the beginning of calculation $(mol \cdot kg(DW)^{-1})$, and

BM is the biomass of the crop $(kg(DW) \cdot m^{-2})$

Content of a certain ion in the crop is:

$$C_{in} = C_{ino} + I_{upt} \cdot DT \quad (mol \cdot m^{-2})$$

where

$$I_{upt} = W_{upt} \cdot C_{soil} \cdot K_{up} \quad (mol \cdot m^{-2} \cdot time^{-1}),$$

I_{upt} is the ion uptake in the crop from the interstitial water,

C_{ino} is the internal content of an ion at beginning of calculation $(mol \cdot m^{-2})$,

W_{upt} is the water uptake (mm or $l(w) \cdot m^{-2}$),

C_{soil} is the calculated soil water concentration of a certain ion as described in Broderson 1984 $(mol \cdot l(w)^{-1})$, and

K_{up} is the uptake coefficient dependent on the crop type and ion (no unit).

The introduction of the uptake coefficient is for calibration purposes and shall be looked upon as a selectivity coefficient with the following description:

$K_{up} > 1$ active ion uptake

$K_{up} = 1$ passive ion uptake

$K_{up} < 1$ selective ion uptake

If the total water uptake per month from a soil is W_{tup}, then the uptake of water from compartment (i) is:

$$W_{upi} = W_{tup} \cdot F_{roi} \quad (mm \cdot month^{-1})$$

Fraction of roots in soil layer:

$$F_{roi} = \sum_{I_i}^{I_j} RDC \quad \text{(decimal fraction)}$$

RDC is the root distribution coefficient.

Calculation of the content of a certain ion on the surface of a crop is calculated in the following way:

$$C_{out} = C_{outo} + (UP_{air} - R_{wof}) \cdot DT \quad (mol \cdot m^{-2})$$

DT is the timestep (e.g., month).

continued...

This wash off rate (R_{wof}) is described in a simple way as a constant wash off coefficient (C_{wof}) multiplied with the surface intercepted content (C_{out}) on the vegetation:

$$R_{wof} = C_{wof} \cdot C_{out} \quad (\mathrm{mol \cdot m^{-2} \cdot time^{-1}})$$

where

C_{wof} is wash of constant (0.037 - 0.054 $\mathrm{day^{-1}}$) (Chamberlain 1970) ($\mathrm{time^{-1}}$), and

C_{out} is the content on the surface of intercepted ions. ($\mathrm{mol \cdot m^{-2}}$).

This description shall be used in the present model as the direct interception of air pollutants as dry and wet deposition on the vegetation. The formulation shall be:

$$UP_{air} = F \cdot DEP \quad (\mathrm{mol \cdot m^{-2} \cdot time^{-1}})$$

$$F = 1 - e^{-My \cdot W} \quad (\text{no unit})$$

where

F is the fraction intercepted on the vegetation,

DEP is the total deposition of the pollutant, calculated from the air pollution model (Hojerup 1984) ($\mathrm{mol \cdot m^{-2} \cdot time^{-1}}$),

My is the filtration parameter with values around 2.3 - 3.3 (Chamberlain 1970) ($\mathrm{m^2 \cdot kg^{-1}}$), and

W is the herbage areal density (dry weight $\cdot\ \mathrm{m^{-2}}$)

Calculation of the root and above ground content of ions, e.g., calcium shall be calculated in the following way:

$$CA_{root} = \frac{CA_{tot}}{(BM/(DCl_{ca} \cdot ORB \cdot ILAG)) + 1} \quad (\mathrm{mol(Ca) \cdot m^{-2}})$$

where

CA_{root} is calcium in the root biomass ($\mathrm{mol(Ca) \cdot m^{-2}}$),

CA_{tot} is the total calcium in root and overground biomass ($\mathrm{mol(Ca) \cdot m^{-2}}$),

BM is the overground biomass of the crop ($\mathrm{kg(DW) \cdot m^{-2}}$),

DCl_{ca} is the distribution coefficient between root/top for calcium in ($\mathrm{mol(Ca) \cdot kg(DW)^{-1}}$ root biomass/($\mathrm{mol(Ca) \cdot kg(DW)^{-1}}$ above ground biomass).

The organic root biomass (ORB) in dry weight for a crop in a certain soil compartment shall be calculated in the following way:

$$ORB = 0.07 \cdot F_{roi} \cdot BM/ILAG \quad (\mathrm{kg(DW) \cdot l(s)^{-1}})$$

BM is the above ground biomass. The use of 0.07 as exchange coefficient for all crops is a rough estimate. This shall be changed when better data is available. ILAG is the depth of the soil layer (mm).

Calculation of the above ground calcium content CA_{veg} is calculated as:

$$CA_{veg} = CA_{tot} - CA_{root} \quad (\mathrm{mol(Ca) \cdot m^{-2}})$$

continued...

Distribution coefficient for calcium $DC1_{ca}$ is 0.5 if the soil water concentration is less than 10^{-5} $mol \cdot L(w)^{-1}$ and 0.1 if the concentration is greater than or equal to 10^{-5} $mol \cdot L(w)^{-1}$. The same distribution coefficients are used for all ions except potassium (K) where a value of 0.5 is used for all concentration levels (Baker 1983).

For cadmium a value of 0.1 is used for potatoes and 0.2 for beets (Coughtrey and Thorne 1983). For other crops the values for calcium are used.

$$CA_{straw} = \frac{CA_{veg}}{(BM_g/(DC2_{ca} \cdot BM_{st})) + 1} \quad (mol(Ca) \cdot m^{-2})$$

where

CA_{veg} is the total Ca content of the overground vegetative biomass ($mol \cdot m^{-2}$),

BM_g is the biomass of grain ($kg(DW) \cdot m^{-2}$),

BM_{st} is the biomass of straw ($kg(DW) \cdot m^{-2}$) and

$DC2_{ca}$ is the distribution coefficient between straw and grain for calcium ($mol(Ca \cdot kg(DW)^{-1}$ straw/$(mol(Ca) \cdot kg(DW)^{-1}$ grain).

Calcium content in grain is then:

$$CA_{grain} = CA_{veg} - CA_{straw} \quad (mol(Ca) \cdot m^{-2})$$

Concentrations are found by division with the grain biomass. It is assumed that 50% of the above ground biomass of cereals is grain.

van Keulen, H. and C.T. de Wit. 1982. A hierarchial approach to agricultural production modelling. In: Proceedings on Modeling Agricultural - Environmental Processes in Crop Production, eds. G. Golubev and I. Shuytov. Collaborative Proceedings Series. CP-82-S5, International Institute for Applied Systems Analysis, Laxenburg, Austria, pp. 139-153.

A listing of the program of the model SUCROS.

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TITLE SUCROS - A SIMPLE AND UNIVERSAL CROP GROWTH SIMULATOR
***      DRY WEIGHT OF PLANT ORGANS, GROWTH RATES AND PARTITIONING

               WLV = INTGRL (WLVI, GLV - DLV)                                   101
               WST = INTGRL (0., GST)                                           102
               WSO = INTGRL (0., GSO)                                           103
               WRT = INTGRL (WRTI, GRT)                                         104
*        WEIGHTS OF LEAF BLADES, STEMS (TRUE STEMS AND LEAF SHEATHS), STORAGE
*              ORGANS AND ROOTS RESP., IN KG/HA
INCON WLVI = 25., WRTI = 25.                                                    105
*        WEIGHT OF LEAVES AND ROOTS AT EMERGENCE

               GTW = (GPHOT - MAINT) * CVF                                      106
*        GROWTH RATE OF ALL ORGANS COMBINED, IN KG/HA/DAY
               GRT = GTW * (1. - FSH)                                           107
               GSH = GTW * FSH                                                  108
               GLV = GSH * FLV                                                  109
               GST = GSH * FST                                                  110
               GSO = GSH * FSO                                                  111
*        GROWTH RATES OF ROOTS AND SHOOTS (LEAVES, STEMS, STORAGE ORGANS)
*              IN KG/HA/DAY
               DLV = WLV * RDR                                                  112
*        DEATH RATE OF LEAVES, IN KG/HA/DAY
               RDR = AFGEN (RDRTB, DVS)                                         113
FUNCTION RDRTB = 0., 0., 1., 0., 1.01, 0.03, 2., 0.03                           114
               WLVD = INTGRL (0., DLV)                                          115
*        DEAD MATERIAL (LEAVES) AT THE FIELD IN KG/HA

               FSH = AFGEN (FSHTB, DVS)                                         116
FUNCTION FSHTB =0., 0.5, 0.3, 0.5, 0.45, 0.775, 0.7, 0.825, 1., 1., 2., 1.      117
*        FRACTION OF GROWTH OCCURRING IN SHOOTS AS FUNCTION OF DEVELOPMENT STAGE
               FLV = AFGEN (FLVTB, DVS)                                         118
               FST = AFGEN (FSTTB, DVS)                                         119
               FSO = 1. - FLV - FST                                             120
FUNCTION FLVTB = 0., 1., 0.45, 1., 0.85, 0., 2., 0.                             121
FUNCTION FSTTB = 0., 0., 0.45, 0., 0.85, 1., 1., 1., 1.01, 0., 2., 0.           122

***      CARBON BALANCE PROCESSES

               LAI = WLV * SLFA                                                 201
PARAM SLFA = 0.0020                                                             202
*        LEAF AREA INDEX IN HA/HA AND SPECIFIC LEAF AREA
*              IN HA LEAF/ KG LEAF WEIGHT

               GPHOT = DTGA * 30. / 44.                                         203
               DTGA = FOV * DGAO + (1. - FOV) * DGAO                            204
*        GROSS PHOTOSYNTHESIS IN KG (CH2O AND CO2 RESP.) PER HA PER DAY,
*              CALCULATED FROM LEAF CHARACTERISTICS (HMAX, EFF), LAI AND ACTUAL
*              DAILY RADIATION (AVRAD), AND CORRECTED FOR DAYLENGTH (DL AND DLE):
               DGAC = INSW (LAI - 5., PHCL, PHCH)                               205
               DGAO = INSW (LAI - 5., PHOL, PHOH)                               206
               PHCH = 0.95 * (PHCH1 + PHCH2) + 20.5                             207
               PHCH1 = SSLAE * AMAX * DLE * X / (1. + X)                        208
               X = ALOG (1. + 0.45 * DRC / (DLE * 3600.) * EFFE / (SSLAE * AMAX))    209
               PHCH2 = (5. - SSLAE) * AMAX * DLE * Y / (1. + Y)                 210
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continued...

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              Y = ALOG (1. + 0.55 * DRC / (DLE * 3600.) * EFFE / ...           211
                 ((5. - SSLAE) * AMAX))                                        211
              SSLAE = SIN ((90. + DEC - LAT) * PI / 180.)                      212
              PHCL = AMIN1 (PHC3, PHC4) * (1. - EXP ((AMAX1 (PHC3, PHC4) / ... 213
                 AMIN1 (PHC3, PHC4))))                                         213
              PHC3 = PHCH * (1. - EXP (-0.8 * LAI))                            214
              PHC4 = DL * LAI * AMAX                                           215
              PHOH = 0.9935 * PHDH1 + 1.1                                      216
              PHOH1 = 5. * AMAX * DLE * Z / (1. + Z)                           217
              Z = DRO / (DLE * 3600.) * EFFE / (5. * AMAX)                     218
              PHOL = AMIN1 (PHO3, PHC4) * (1. - EXP (- (AMAX1 (PHO3, PHC4) / ... 219
                 AMIN1 (PHO3, PHC4))))                                         219
              PHO3 = PHOH * (1. - EXP (-0.8 * LAI))                            220
              EFFE = (1. - REFLC) * EFF                                        221
PARAM EFF = 0.5, AMAX = 3.0, REFLC = .08                                       221
*        INITIAL LIGHT USE EFFICIENCY AND LIGHT SATURATED CO2 ASSIMILATION
*             RATE OF INDIVIDUAL LEAVES.  UNITS: KG CO2/ HA/ HR / (J/ M2/ S) AND
*             KG CO2/HA LEAF/HR
              FOV = (DRC - AVRAD) / (0.8 * DRC)                                222
*        AVERAGE FRACTION OF PERIOD OVERCAST DURING A DAY.
*             CALCULATION OF DAILY RADIATION OF A CLEAR AND AN OVERCAST SKY (DRC
*             AND DRO, P.A.R., IN J/M2) AND OF DAYLENGTH (IN HR) AS A FUNCTION OF
*             LATITUDE (LAT, IN DEGREE), DECLINATION (DEC, IN DEGREE) AND DATE:
              DRC = 0.5 * 1300. * RDN * EXP (-0.1 / (RDN / (DL * 3600.)))     223
              DRO = 0.2 * DRC                                                  224
              RDN = 3600. * (SINLD * DL + 24. / PI * COSLD * SQRT (1. - ...    225
                 (SINLD / COSLD) ** 2))                                        225
              SINLD = SIN (DEC * PI / 180.) * SIN (LAT * PI / 180.)            226
              COSLD = COS (DEC * PI / 180.) * COS (LAT * PI / 180.)            227
              DEC = -23.4 * COS (2. * PI * (DAY + 10.) / 365.)                 228
              DL = 12. * (PI + 2. * ASIN (SINLD/COSLD)) / PI                   229

              DLE = 12. * (PI + 2. * ASIN ((-SIN (8. * PI / 180) + SINLD) / ... 230
                 COSLD)) / PI                                                  230
              DLP = 12. * (PI + 2. * ASIN ((-SIN (-4. * PI / 180.) + SINLD) / ... 231
                 COSLD)) / PI                                                  231
CONSTANT PI = 3.1416                                                           232
PARAM LAT = -15.                                                               233

*        MAINTENANCE RESPIRATION
              MAINT = AMIN1 (GPHOT, MAINTS * TEFF)                             234
              MAINTS = WLV * 0.03 + WST * 0.015 + WSO * 0.01 + WRT * 0.01      235
              TEFF = Q10 ** (0.1 * TMPA - 2.5)                                 236
PARAM Q10 = 2.                                                                 237

*        GROWTH EFFICIENCY
              CVF = (FLV * 0.72 + FST * 0.69 + FSO * CVFSO) * FSH + ...        238
                 (1. - FSH) * 0.72                                             238
PARAM CVFSO = 0.73                                                             239

***      DEVELOPMENT OF THE VEGETATION

              DVS = INTGRL (0., INSW (DVS - 1., DVRV, DVRR))                   301
FINISH DVS = 2.                                                                302
              DVRV = 0.0252 * AFGEN (DVRTTB, TMPA) * AFGEN (DVRDTB, DLP)       303
              DVRR = 0.0477 * AFGEN (DVRRTB, TMPA)                             304
FUNCTION DVRTTB = 10., .63, 15., .83, 20., .92, 25., .96, 30., .98, ...        305
                 35., .99                                                      305
FUNCTION DVRRTB = 10., .08, 15., .38, 20., .575, 25., .71, 30., .80, ...       306
                 35., .865                                                     306
FUNCTION DVRDTB = 10., 0.223, 11., 0.425, 12.0, 0.575, 13., 0.685, ...         307
                 14., 0.767, 15., 0.828, 16., 0.872, 17., 0.906                307
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continued...

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***      WEATHER DATA
                  DAY = AMOD (TIME, 365.)                                          401
                  AVRAD = 0.5 * 41820. * AFGEN (AVRADT, DAY)                       402
FUNCTION AVRADT = 1., 523., 15., 526., 46., 532., 74., 575., 105., ...             403
                  557., 135., 509., 166., 466., 196., 482., 227., 545., 258., ...  403
                  611., 288., 644., 319., 556., 349., 521., 365., 523.             403

TMPA = 0.5 * (AFGEN (TMAXT, DAY) + AFGEN (TMINT, DAY))                             404
FUNCTION TMAXT = 1., 28.6, 15., 28.3, 46., 28.1, 74., 28.7, 105., ...              405
                  28.9, 135., 27.2, 166., 24.9, 196., 24.7, 227., 27.4, 258., ...  405
                  29.9, 288., 33.6, 319., 31.3, 349., 28.9, 365., 28.6             405
FUNCTION TMINT = 1., 18.2, 15., 18.2, 46., 18.2, 74., 16.3, 105., ...              406
                  13.9, 135., 10.1, 166., 8.5, 196., 7.4, 227., 9.7, 258., ...     406
                  13.4, 288., 16.6, 319., 18.2, 349., 18.2, 365., 18.2             406

***      SIMULATION RUN SPECIFICATIONS
TIMER FINTIM = 1000., DELT = 2., PRDEL = 2., OUTDEL = 2., TIME = 300.              501

*        INITIAL VALUE OF TIME INDICATES STARTING DAY OF SIMULATION
METHOD RKSFX                                                                       502
PRINT WLV, WLVD, WST, WSO, WRT, LAI, DVS, MAINT, DTGA, CVF                         503
              NWRT = -WRT                                                          504
              WLVT = WLV + WLVD                                                    505
              WVEG = WLVT + WST                                                    506
              TADRW = WVEG + WSO                                                   507
PRTPLOT NWRT, WLV, WLVT, WVEG, TADRW                                               508
PAGE GROUP, NPLOT = 5                                                              509
END
STOP
ENDJOB
```

An explanation of the abbreviations used in the model SUCROS as listed.

NAME	DESCRIPTION	UNIT
AMAX	CO2 ASSIMILATION RATE OF A LEAF AT LIGHT SATURATION	KG (CO2)/ HA (LEAF)/ H
AVRAD	ACTUAL DAILY RADIATION (400-700 NM)	J/M2/D
AVRADT	TABLE MEASURED GLOBAL RADIATION (CAL/ CM2/ D) VS. DAYNUMBER	-
CVF	CONVERSION EFFICIENCY FOR GROWTH OF PLANT DRY MATTER	KG (DM)/ KG (CH2O)
CVFSO	CONVERSION EFFICIENCY FOR FORMATION OF STORAGE ORGANS	KG (DM)/ KG (CH2O)
DAY	NUMBER OF DAYS IN THE YEAR FROM 1ST OF JANUARY	DAY
DEC	DECLINATION OF SUN WITH RESPECT TO THE EQUATOR	DEGREE
DGAC	DAILY GROSS CO2 ASSIMILATION -CLEAR SKY-	KG (CO2)/ HA/ D
DGAO	DAILY GROSS CO2 ASSIMILATION -OVERCAST SKY-	KG (CO2)/ HA/ D
DL	ASTRONOMICAL DAYLENGTH	H
DLE	EFFECTIVE DAYLENGTH	H
DLP	PHOTOPERIODIC DAYLENGTH	H
DLV	DEATH RATE OF THE LEAVES	KG/ HA/ D
DRC	PHOTOSYNTHETICALLY ACTIVE RADIATION -STANDARD CLEAR SKY-	J/ M2/ D
DRO	PHOTOSYNTHETICALLY ACTIVE RADIATION -STANDARD OVERCAST SKY-	J/ M2/ D
DTGA	ACTUAL DAILY GROSS CO2 ASSIMILATION	KG (CO2)/ HA/ D
DVRDTB	RELATION BETWEEN RATE OF DEVELOPMENT AND DAYLENGTH	-
DVRR	RATE OF DEVELOPMENT IN REPRODUCTIVE PHASE IN RELATION TO TEMPERATURE	1/D
DVRRTB	TABLE OF DVRR AS FUNCTION OF TEMPERATURE	-
DVRTTB	RELATION BETWEEN RATE OF DEVELOPMENT AND TEMPERATURE	-
DVRV	RATE OF DEVELOPMENT IN VEGETATIVE PHASE IN RELATION TO TEMPERATURE AND DAYLENGTH	1/D
DVS	DEVELOPMENT STAGE OF THE CROP	FRACTION
EFF	EFFICIENCY OF USE OF ABSORBED VISIBLE RADIATION FOR CO2 ASSIMILATION AT LOW LIGHT LEVELS	KG (CO2)/ J/ HA/ H M2S
EFFE	EFF BASED ON INCIDENT RADIATION	KG (CO2)/ J/ HA/ H M2S
FLV	FRACTION OF LEAVES IN SHOOT BIOMASS	-
FLVTB	TABLE FLV VS. DEVELOPMENT STAGE	-
FOV	FRACTION OF TIME THAT SKY IS OVERCAST	-
FSH	FRACTION OF SHOOT IN TOTAL PLANT BIOMASS	-
FSHTB	TABLE FSH VS. DEVELOPMENT STAGE	-
FSO	FRACTION OF STORAGE ORGANS IN SHOOT BIOMASS	-
FSOTB	TABLE FSO VS. DEVELOPMENT STAGE	-
FST	FRACTION OF STEMS IN SHOOT BIOMASS	-
FSTTB	TABLE FST VS. DEVELOPMENT STAGE	-
GLV	GROWTH RATE OF THE LEAVES	KG (DM)/ HA/ D
GPHOT	DAILY GROSS CO2 ASSIMILATION	KG (CH2O)/ HA/ D
GRT	GROWTH RATE OF THE ROOTS	KG (DM)/ HA/ D
GSH	GROWTH RATE OF THE SHOOT	KG (DM)/ HA/ D
GSO	GROWTH RATE OF THE STORAGE ORGANS	KG (DM)/ HA/ D
GST	GROWTH RATE OF THE STEMS	KG (DM)/ HA/ D
GTW	GROWTH RATE OF TOTAL PLANT BIOMASS	KG (DM)/ HA/ D
LAI	LEAF AREA INDEX	M2/M2
LAT	LATITUDE	DEGREE
MAINT	MAINTENANCE RESPIRATION OF THE VEGETATION	KG (CH2O)/ HA/ D
MAINTS	MAINTENANCE RESPIRATION AT STANDARD TEMPERATURE (25°C)	KG (CH2O)/ HA/ D

continued...

NAME	DESCRIPTION	UNIT
NWRT	NEGATIVE WEIGHT OF ROOTS (OUTPUT VARIABLE)	KG (DM)/ HA
PI	CIRCUMFERENCE OF A CIRCLE, DIVIDED BY ITS DIAMETER	-
Q10	INCREASE IN RATE OF MAINTENANCE PROCESSES PER 10 DEGREES C	-
RDN	AVERAGE LEVEL INCOMING PHOTOSYNTHETIC ACTIVE RADIATION	J/ M2/ S
RDR	RELATIVE DEATH RATE OF THE LEAVES	1/D
RDRTB	TABLE RDR VS. DEVELOPMENT STAGE	-
REFLC	REFLECTION COEFFICIENT OF THE CANOPY	(FRACTION)
SLFA	SPECIFIC LEAF AREA	HA (LEAF)/ KG (LEAF)
TADRW	TOTAL ABOVE-GROUND BIOMASS	KG/HA
TEFF	EFFECT OF TEMPERATURE ON RATE OF MAINTENANCE RESPIRATION	-
TIME	SIMULATED TIME	DAY
TMAXT	TABLE MAXIMUM TEMPERATURE VS. DAYNUMBER	-
TMINT	TABLE MINIMUM TEMPERATURE VS. DAYNUMBER	-
TMPA	AVERAGE AIR TEMPERATURE	DEGREE C
WLV	WEIGHT OF THE GREEN LEAVES	KG/HA
WLVD	WEIGHT OF THE DEAD LEAVES	KG/HA
WLVI	INITIAL WEIGHT OF THE LEAVES	KG/HA
WLVT	WEIGHT OF THE GREEN PLUS DEAD LEAVES (OUTPUT VARIABLE)	KG/HA
WRT	WEIGHT OF THE ROOTS	KG/HA
WRTI	INITIAL WEIGHT OF THE ROOTS	KG/HA
WSO	WEIGHT OF THE STORAGE ORGANS	KG/HA
WST	WEIGHT OF THE STEMS	KG/HA
WVEG	WEIGHT OF THE VEGETATIVE PARTS (OUTPUT VARIABLE)	KG/HA

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